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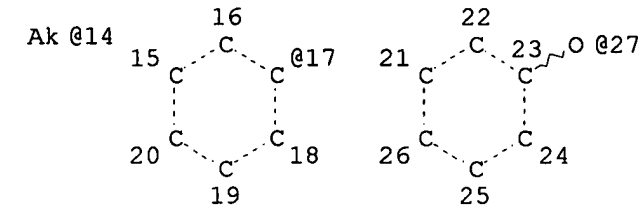
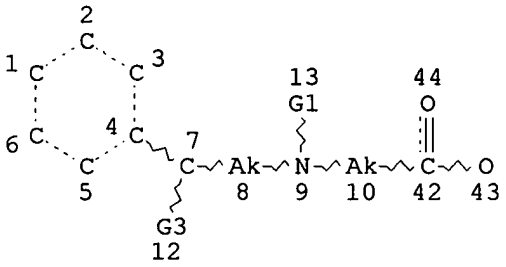
L25 STR





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VAR G3=17/27
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CONNECT IS E1 RC AT 14
DEFAULT MLEVEL IS ATOM
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GGCAT IS LIN LOC AT 10
GGCAT IS LIN LOC SAT AT 14
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 15 21 4
NUMBER OF NODES IS 29

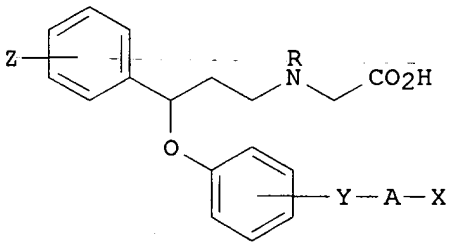
STEREO ATTRIBUTES: NONE
L27 252 SEA FILE=REGISTRY SUB=L9 SSS FUL L25
L28 26 SEA FILE=HCAPLUS ABB=ON PLU=ON L27

L28 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:10422 HCAPLUS
DN 136:70085
TI Preparation of amino acid benzophenone and sulfone derivatives as inhibitors of glycine uptake
IN Lowe, John Adams, III
PA Pfizer Products Inc., USA
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002000602	A1	20020103	WO 2001-IB1139	20010622

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-215692 P 20000630
OS MARPAT 136:70085
GI



I

AB Compds. I [A is Ph, naphthyl, benzothienyl, benzofuranyl, thienyl; a monocyclic aryl or heteroaryl ring contg. 0-4 heteroatoms or a bicyclic aryl or heteroaryl ring contg. 0-5 heteroatoms not contg. any adjacent ring oxygen atoms; Y is CO or SO2 and is attached to the phenoxy group at the meta or para position; X and Z are H, (C1-C6) alkyl or alkoxy optionally substituted with 1-7 fluorine atoms, carboxy, carbalkoxy,carboxamido, alkylthio, sulfoxyl, sulfonyl, halo, nitro, cyano, amino, alkylamino or dialkylamino; R is H, alkyl, preferably Me] or their pharmaceutically acceptable salts were prepd. The title compds. exhibit activity as glycine transport inhibitors and thus can be used for the enhancement of cognition and the treatment of the pos. and neg. symptoms of schizophrenia and other psychoses in mammals, including humans. Thus, [[3-(4-benzoylphenoxy)-3-phenylpropyl]methylamino]acetic acid was prepd. by reaction of 3-chloro-1-bromo-1-phenylpropane with 4-benzoylphenol and sarcosine Et ester hydrochloride, followed by sapon.

IT **385435-93-8P 385435-94-9P 385435-95-0P**
385435-96-1P 385435-97-2P 385435-98-3P
385435-99-4P 385436-00-0P 385436-01-1P
385436-02-2P 385436-03-3P 385436-04-4P
385436-05-5P 385436-06-6P 385436-07-7P
385436-09-9P 385436-10-2P 385436-12-4P
385436-14-6P 385436-16-8P 385436-18-0P
385436-20-4P 385436-25-9P 385436-27-1P
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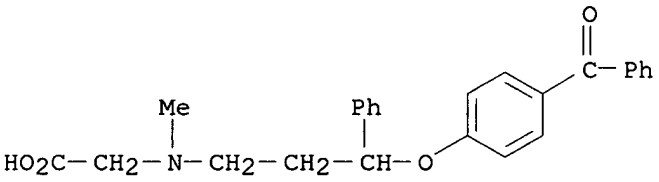
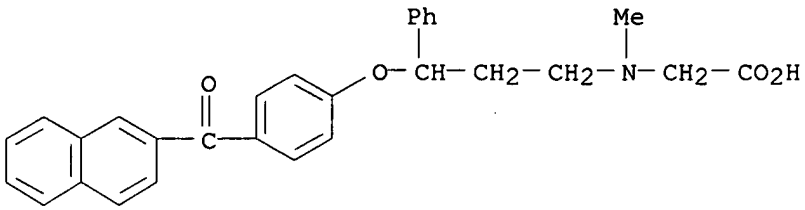
385436-76-0P 385436-77-1P 385436-78-2P
385436-79-3P 385436-80-6P 385436-81-7P
385436-82-8P 385436-83-9P 385436-84-0P
385436-85-1P 385436-86-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid benzophenone and sulfone derivs. as inhibitors of glycine uptake)

RN 385435-93-8 HCAPLUS
CN Glycine, N-[3-(4-benzoylphenoxy)-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



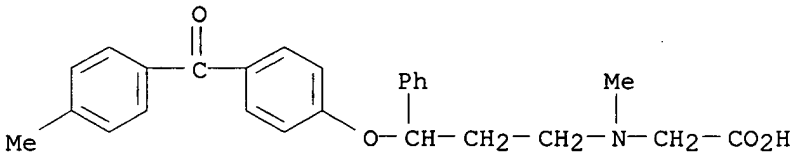
● HCl

RN 385435-94-9 HCAPLUS
CN Glycine, N-methyl-N-[3-[4-(2-naphthalenylcarbonyl)phenoxy]-3-phenylpropyl]-, hydrochloride (9CI) (CA INDEX NAME)



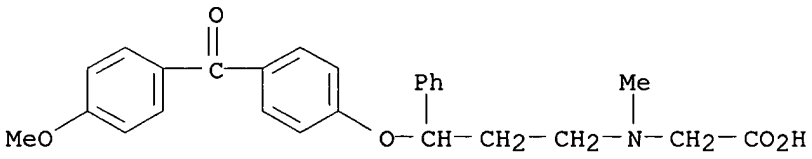
● HCl

RN 385435-95-0 HCAPLUS
CN Glycine, N-methyl-N-[3-[4-(4-methylbenzoyl)phenoxy]-3-phenylpropyl]-, hydrochloride (9CI) (CA INDEX NAME)



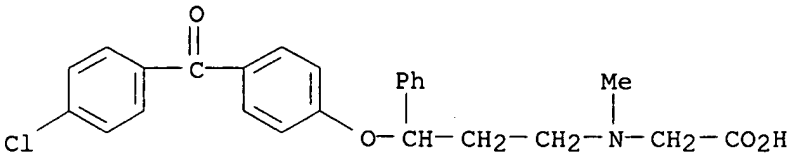
● HCl

RN 385435-96-1 HCAPLUS
CN Glycine, N-[3-[4-(4-methoxybenzoyl)phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



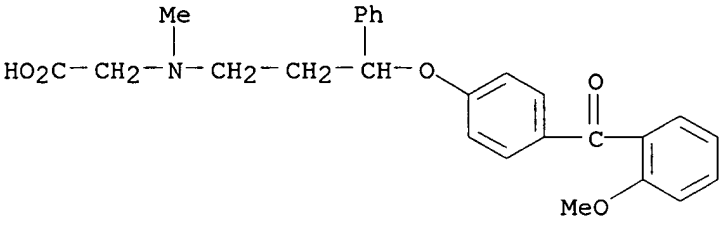
● HCl

RN 385435-97-2 HCAPLUS
CN Glycine, N-[3-[4-(4-chlorobenzoyl)phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



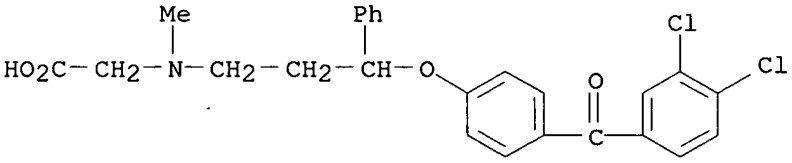
● HCl

RN 385435-98-3 HCAPLUS
CN Glycine, N-[3-[4-(2-methoxybenzoyl)phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



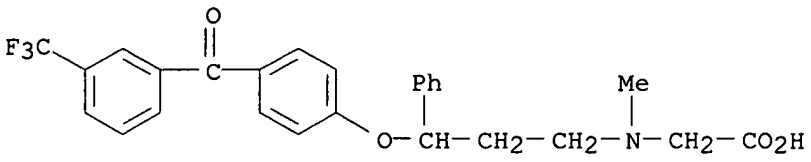
● HCl

RN 385435-99-4 HCAPLUS
CN Glycine, N-[3-[4-(3,4-dichlorobenzoyl)phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



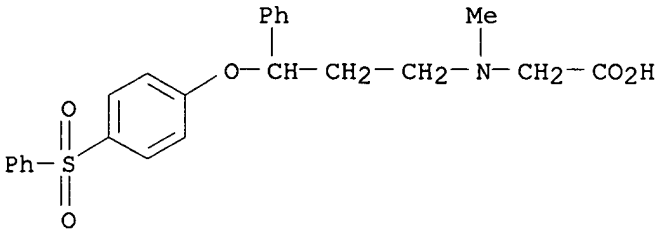
● HCl

RN 385436-00-0 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-[3-(trifluoromethyl)benzoyl]phenoxy]propyl]-, hydrochloride (9CI) (CA INDEX NAME)



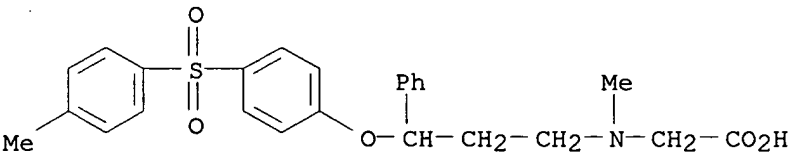
● HCl

RN 385436-01-1 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-(phenylsulfonyl)phenoxy]propyl]-, hydrochloride (9CI) (CA INDEX NAME)



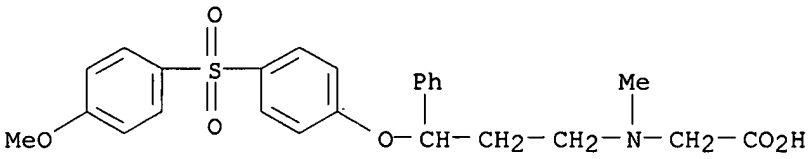
● HCl

RN 385436-02-2 HCAPLUS
CN Glycine, N-methyl-N-[3-[4-[(4-methylphenyl)sulfonyl]phenoxy]-3-phenylpropyl]-, hydrochloride (9CI) (CA INDEX NAME)



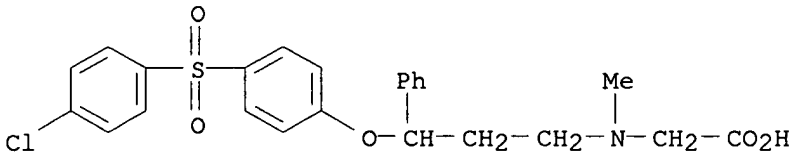
● HCl

RN 385436-03-3 HCAPLUS
CN Glycine, N-[3-[4-[(4-methoxyphenyl)sulfonyl]phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



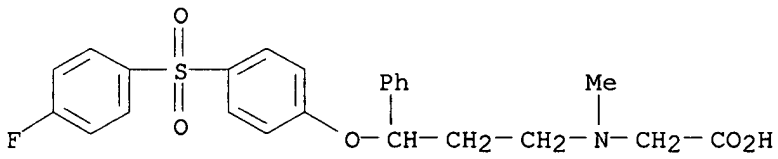
● HCl

RN 385436-04-4 HCAPLUS
CN Glycine, N-[3-[4-[(4-chlorophenyl)sulfonyl]phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



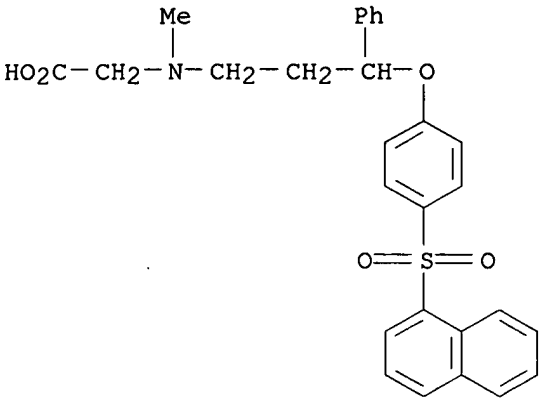
● HCl

RN 385436-05-5 HCAPLUS
CN Glycine, N-[3-[4-[(4-fluorophenyl)sulfonyl]phenoxy]-3-phenylpropyl]-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



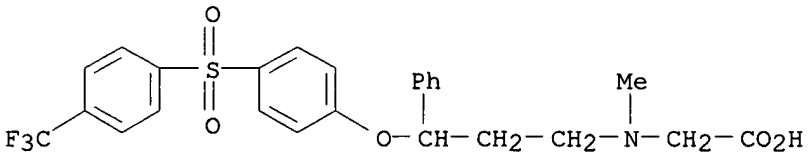
● HCl

RN 385436-06-6 HCAPLUS
CN Glycine, N-methyl-N-[3-[4-(1-naphthalenylsulfonyl)phenoxy]-3-phenylpropyl]-, hydrochloride (9CI) (CA INDEX NAME)



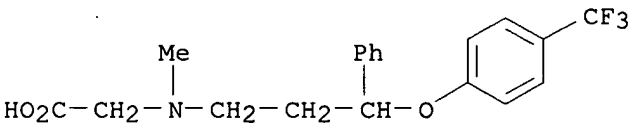
● HCl

RN 385436-07-7 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-[[4-(trifluoromethyl)phenyl]sulfonyl]phenoxy]propyl]-, hydrochloride (9CI) (CA INDEX NAME)

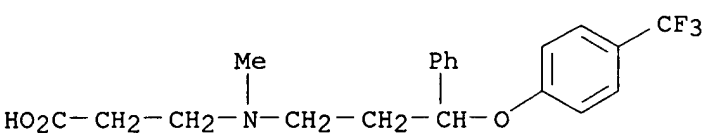


● HCl

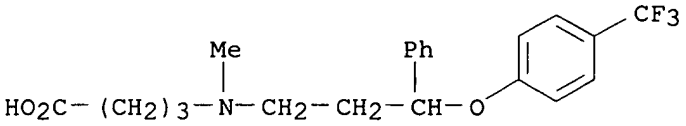
L28 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:501948 HCAPLUS
DN 135:352325
TI Discovery and SAR of Org 24598-A Selective Glycine Uptake Inhibitor
AU Brown, A.; Carlyle, I.; Clark, J.; Hamilton, W.; Gibson, S.; McGarry, G.; McEachen, S.; Rae, D.; Thorn, S.; Walker, G.
CS Department of Medicinal Chemistry, Organon Research and Development Group, Newhouse, Lanarkshire, ML1 5SH, UK
SO Bioorganic & Medicinal Chemistry Letters (2001), 11(15), 2007-2009
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB The authors describe the discovery of a series of selective GlyT-1b inhibitors, by application of solid-phase chem. and library design. Specifically the discovery of Org 24598, one of the first potent and selective inhibitors of the glycine transporter is discussed. In vitro structure-activity relationships (SARs) data for interaction of a ligand with this system is discussed.
IT **372198-80-6P**, Org 24461 **372198-81-7P**, Org 24629
372198-82-8P, Org 24628 **372198-83-9P**, Org 24660
372198-85-1P, Org 24658 **372198-86-2P**, Org 24668
372198-87-3P, Org 24667 **372198-88-4P**, Org 24642
372198-89-5P, Org 24641 **372198-90-8P**, Org 24872
372198-91-9P, Org 24730 **372198-92-0P**, Org 24520
372198-93-1P, Org 24747 **372198-94-2P**, Org 24669
372198-95-3P, Org 24645 **372198-96-4P**, Org 24706
372198-97-5P, Org 24598 **372198-98-6P**, Org 24597
372198-99-7P, Org 24835 **372199-00-3P**, Org 24836
372199-01-4P, Org 24915 **372199-02-5P**, Org 24914
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of N-substituted glycine derivs. as selective inhibitors of the glycine transporter)
RN 372198-80-6 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (9CI) (CA INDEX NAME)



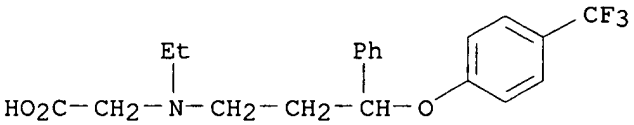
RN 372198-81-7 HCAPLUS
CN .beta.-Alanine, N-methyl-N-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (9CI) (CA INDEX NAME)



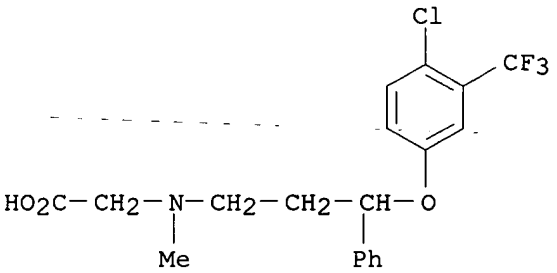
RN 372198-82-8 HCAPLUS
CN Butanoic acid, 4-[methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]amino]- (9CI) (CA INDEX NAME)



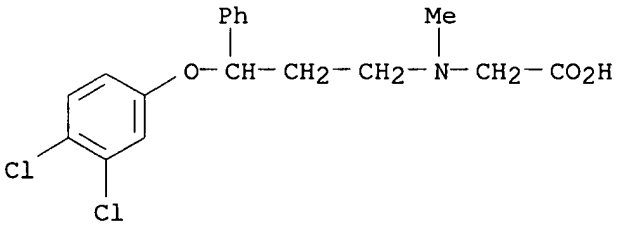
RN 372198-83-9 HCAPLUS
CN Glycine, N-ethyl-N-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (9CI) (CA INDEX NAME)



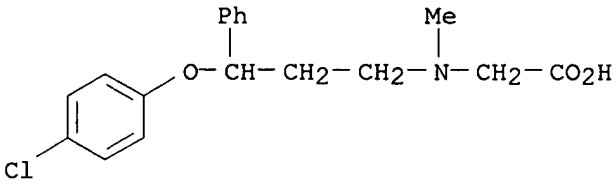
RN 372198-85-1 HCAPLUS
CN Glycine, N-[3-[4-chloro-3-(trifluoromethyl)phenoxy]-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



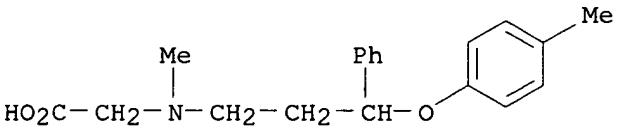
RN 372198-86-2 HCAPLUS
CN Glycine, N-[3-(3,4-dichlorophenoxy)-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



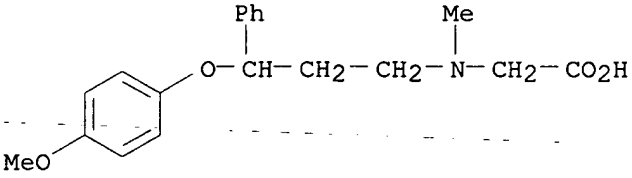
RN 372198-87-3 HCAPLUS
CN Glycine, N-[3-(4-chlorophenoxy)-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



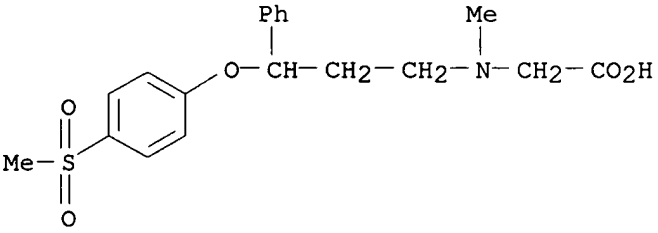
RN 372198-88-4 HCAPLUS
CN Glycine, N-methyl-N-[3-(4-methylphenoxy)-3-phenylpropyl]- (9CI) (CA INDEX NAME)



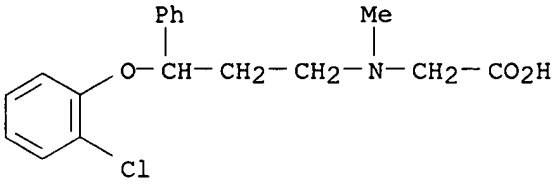
RN 372198-89-5 HCAPLUS
CN Glycine, N-[3-(4-methoxyphenoxy)-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



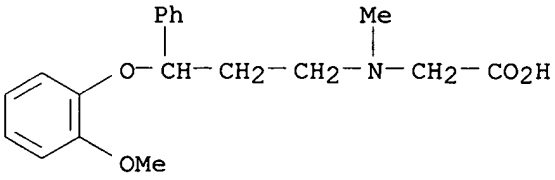
RN 372198-90-8 HCAPLUS
CN Glycine, N-methyl-N-[3-[4-(methylsulfonyl)phenoxy]-3-phenylpropyl]- (9CI) (CA INDEX NAME)



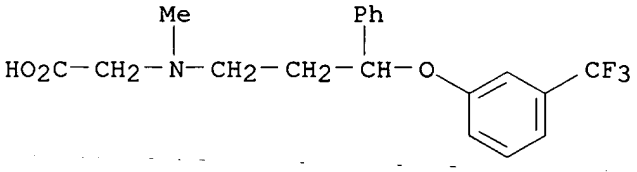
RN 372198-91-9 HCAPLUS
CN Glycine, N-[3-(2-chlorophenoxy)-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



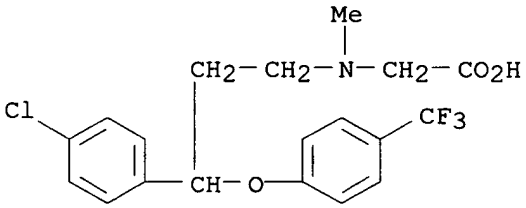
RN 372198-92-0 HCAPLUS
CN Glycine, N-[3-(2-methoxyphenoxy)-3-phenylpropyl]-N-methyl- (9CI) (CA INDEX NAME)



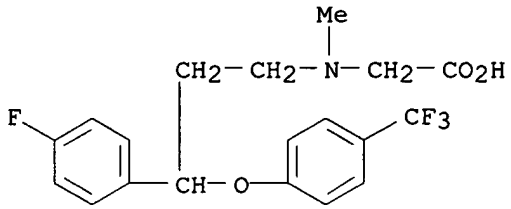
RN 372198-93-1 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[3-(trifluoromethyl)phenoxy]propyl]- (9CI) (CA INDEX NAME)



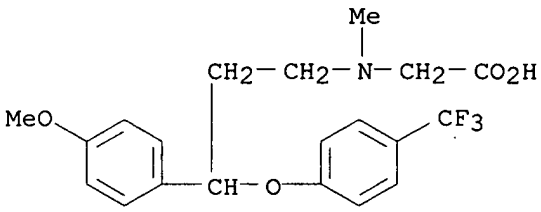
RN 372198-94-2 HCAPLUS
CN Glycine, N-[3-(4-chlorophenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 372198-95-3 HCAPLUS
CN Glycine, N-[3-(4-fluorophenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 372198-96-4 HCAPLUS
CN Glycine, N-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]-N-methyl- (9CI) (CA INDEX NAME)

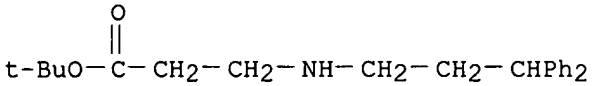


L28 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:338559 HCAPLUS
DN 134:340710
TI Preparation of peptides as HCV NS3 protease inhibitors
IN Fattori, Daniela; Pessi, Antonello; Ingallinella, Paolo; Bianchi, Elisabetta
PA Istituto di Ricerche di Biologia Molecolare P. Angeletti S.p.A., Italy; Nicholls, Kathryn, M.
SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001032691	A1	20010510	WO 2000-GB4195	20001102

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

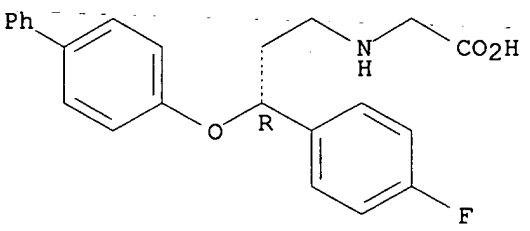
PRAI GB 1999-25955 A 19991102
OS MARPAT 134:340710
AB Peptides HO2C-X-CONHCH(A)CON(B)CH(D)(CH2)pCO-X [X represents a benzene or non-arom. carbocyclic ring having 4-8 carbon atoms; A = cyclohexylmethyl or optionally substituted phenyl; B = H, alkyl, aralkyl; D = H, CONHCH(Bu-i)COR (R = OH, alkylamino, or cycloalkylamino), CONHCH2Bu-i, in which each stereo-center is in the R or S configuration; p = 1 or 2; X = OH, alkoxy] or their pharmaceutically acceptable salts and esters were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, HO2C-X-CO-Cha-Asp-Leu-NH2 (R,R,S,S,S and S,S,S,S,S-diastereomers; X = 1,2-cyclohexanediyl, Cha = cyclohexylalanine), prepd. by std. solid-phase peptide coupling, showed IC50 = 15 and 54 .mu.M, resp., for inhibition of HCV NS3 protease.
IT **337953-80-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptides as HCV NS3 protease inhibitors)
RN 337953-80-7 HCAPLUS
CN .beta.-Alanine, N-(3,3-diphenylpropyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

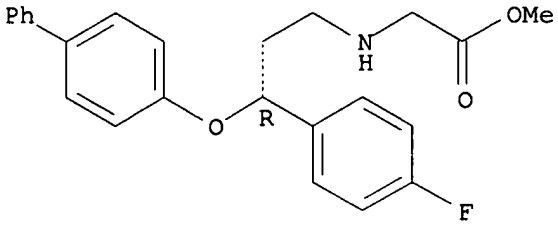
L28 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:151111 HCAPLUS
DN 134:311410
TI Radiosynthesis of a ligand for studying the glycine transporter: [11C]ALX-5407
AU Ravert, Hayden T.; Mathews, William B.; Klitenick, Mark A.; Wong, Dean F.; Dannals, Robert F.
CS Division of Nuclear Medicine, Department of Radiology, The Johns Hopkins Medical Institutions, Baltimore, MD, 21287-0750, USA
SO J. Labelled Compd. Radiopharm. (2001), 44(3), 241-246
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB [11C]ALX-5407, R-N[3-(4'-fluorophenyl)-3-(4'-phenylphenoxy)propyl] sarcosine, a chiral glycine transporter 1 antagonist, was labeled with [11C]iodomethane by N-alkylation of Me ester protected N-normethyl precursor, ALX-5536, and subsequent sapon. of the Me ester protecting group. The time for synthesis, purifn., and formulation was 33 min with an av. specific radioactivity of 3909 mCi/.mu.mol (EOS) and av. decay cor. radiochem. yield of 8%.
IT **335427-27-5P**, Saponified ALX 5536
RL: BYP (Byproduct); PREP (Preparation)
(radiosynthesis of glycine transporter antagonist [11C]ALX-5407)
RN 335427-27-5 HCAPLUS
CN Glycine, N-[(3R)-3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



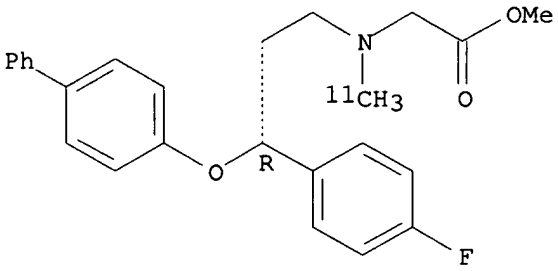
IT **335259-71-7**, ALX 5536 **335259-72-8**, ALX 5406
RL: RCT (Reactant)
(radiosynthesis of glycine transporter antagonist [11C]ALX-5407)
RN 335259-71-7 HCAPLUS
CN Glycine, N-[(3R)-3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



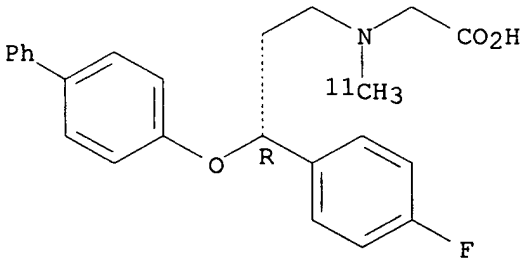
RN 335259-72-8 HCAPLUS
CN Glycine, N-[(3R)-3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]-N-(methyl-11C)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **335259-73-9P**, ALX 5407
RL: SPN (Synthetic preparation); PREP (Preparation)
(radiosynthesis of glycine transporter antagonist [11C]ALX-5407)
RN 335259-73-9 HCAPLUS
CN Glycine, N-[(3R)-3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]-N-(methyl-11C)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



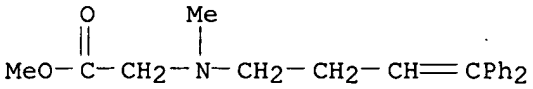
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:132748 HCAPLUS
DN 134:178816
TI Preparation of amino acid derivatives as pharmaceuticals for treatment of neurological and neuropsychiatric disorders
IN Ognyanov, Vassil Iliya; Borden, Laurence A.; Bell, Stanley Charles; Zhang, Jing
PA Allelix Neuroscience Inc., USA
SO U.S., 52 pp., Cont.-in-part of U. S. Ser. No.656,063, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

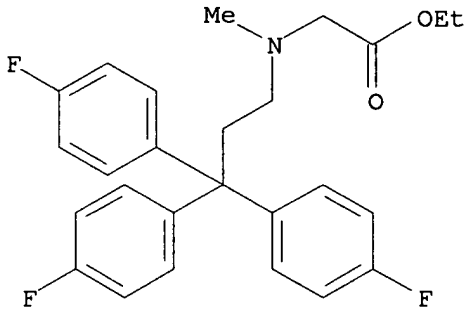
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6191165	B1	20010220	US 1997-866007	19970530
	US 2001012857	A1	20010809	US 2001-757011	20010109
PRAI	US 1996-41503	P	19960531		
	US 1996-41504	P	19960531		
	US 1996-655912	B2	19960531		
	US 1996-656063	B2	19960531		
	US 1997-44387	P	19970227		
	US 1997-70900	P	19970227		
	US 1997-808754	B2	19970227		
	US 1997-808755	A2	19970227		
	US 1997-807682	A2	19970228		
	US 1997-866007	A3	19970530		

OS MARPAT 134:178816
AB Amino acid derivs. R2RxRyXR1NR3(R3*)nCR4R4*R5 [X = N, C (R2 not present when X = N); R2 = H, alkyl, alkoxy, cyano, alkanoyl, etc.; Rx, Ry = aryl, heteroaryl, adamantyl, or nonarom. ring linked to X via a single bond, alkylene, etc.; R1 = alkylene, iminooxyethylene, etc.; R3 = H, alkyl, (un)substituted Ph or phenylalkyl, etc.; R3* = alkyl, O; n = 0, 1; R4, R4* = H, alkyl, hydroxyalkyl; R5 = (un)substituted carbamoyl, carboxy, aminosulfonyl, phosphoryl, etc.] were prepd. as pharmaceuticals for treatment of neurol. and neuropsychiatric disorders. Thus, N-(4,4-diphenyl-3-butenyl)glycine Et ester was by alkylation of glycine Et ester hydrochloride with 4-bromo-1,1-diphenyl-1-butene. Binding assays to measure interaction of compds. with the glycine site on the NMDA receptor are illustrated.
IT **200004-42-8P 200004-51-9P 200004-53-1P**
200004-54-2P 200004-56-4P 200004-58-6P
200004-59-7P 200004-66-6P 200004-67-7P
200004-70-2P 200004-71-3P 200004-73-5P
200004-75-7P 200004-76-8P 200004-77-9P
200004-78-0P 200004-79-1P 200004-80-4P
200004-81-5P 200004-84-8P 200004-90-6P
200004-96-2P 200005-05-6P 200005-07-8P
200005-08-9P 200005-11-4P 200005-17-0P
200005-34-1P 200005-46-5P 200005-51-2P
200005-52-3P 200005-54-5P 200006-07-1P
200006-08-2P 200006-09-3P 200006-10-6P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid derivs. as pharmaceuticals for treatment of

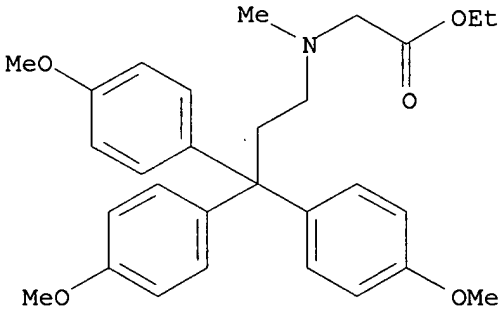
neurol. and neuropsychiatric disorders)
RN 200004-42-8 HCAPLUS
CN Glycine, N-(4,4-diphenyl-3-butenyl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



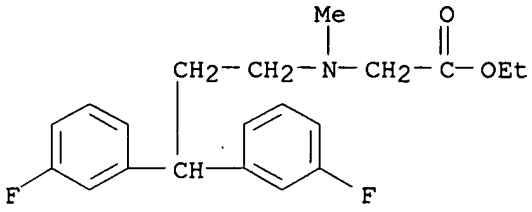
RN 200004-51-9 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-fluorophenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)



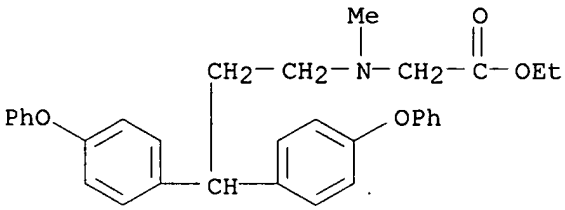
RN 200004-53-1 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-methoxyphenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)



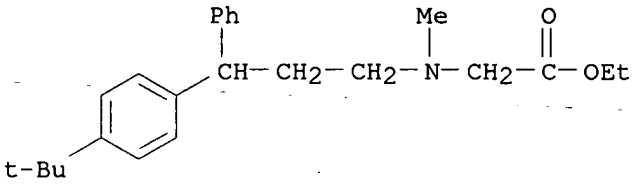
RN 200004-54-2 HCAPLUS
CN Glycine, N-[3,3-bis(3-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



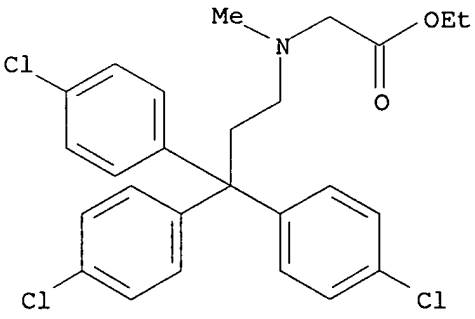
RN 200004-56-4 HCAPLUS
CN Glycine, N-[3,3-bis(4-phenoxyphenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



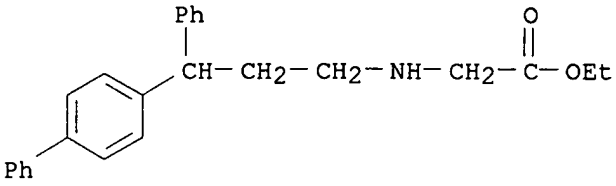
RN 200004-58-6 HCAPLUS
CN Glycine, N-[3-[4-(1,1-dimethylethyl)phenyl]-3-phenylpropyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



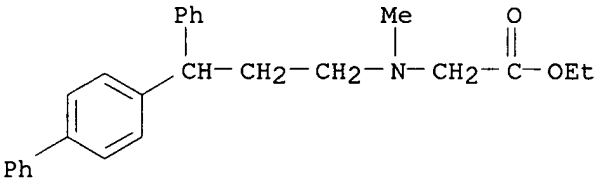
RN 200004-59-7 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-chlorophenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)



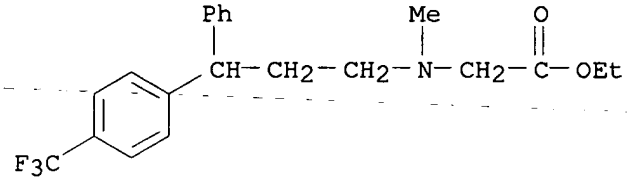
RN 200004-66-6 HCAPLUS
CN Glycine, N-(3-[1,1'-biphenyl]-4-yl-3-phenylpropyl)-, ethyl ester (9CI) (CA INDEX NAME)



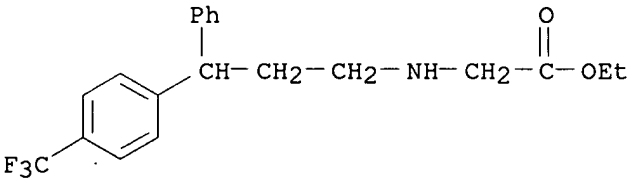
RN 200004-67-7 HCAPLUS
CN Glycine, N-(3-[1,1'-biphenyl]-4-yl-3-phenylpropyl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



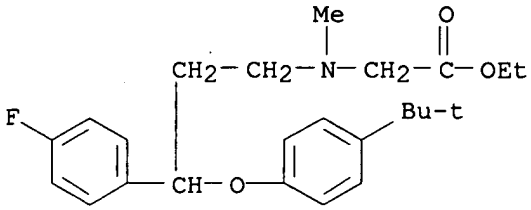
RN 200004-70-2 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-(trifluoromethyl)phenyl]propyl]-, ethyl ester (9CI) (CA INDEX NAME)



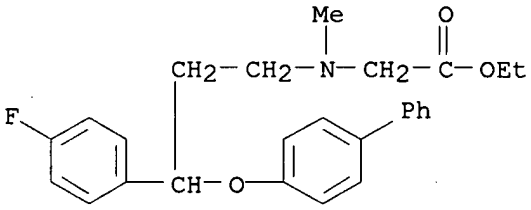
RN 200004-71-3 HCAPLUS
CN Glycine, N-[3-phenyl-3-[4-(trifluoromethyl)phenyl]propyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 200004-73-5 HCAPLUS
CN Glycine, N-[3-[4-(1,1-dimethylethyl)phenoxy]-3-(4-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 200004-75-7 HCAPLUS
CN Glycine, N-[3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1997:803807 HCAPLUS
DN 128:48490
TI Preparation of amino acid derivatives as pharmaceuticals for treatment of neurological and neuropsychiatric disorders
IN Ognyanov, Vassil Iliya; Borden, Laurence; Bell, Stanley Charles; Zhang, Jing
PA Trophix Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9745115	A1	19971204	WO 1997-US9450	19970529
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	AU 9731530	A1	19980105	AU 1997-31530	19970529
	AU 730789	B2	20010315		
	EP 1014966	A1	20000705	EP 1997-926871	19970529
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
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	CN 1327383	A	20011219	CN 1997-196821	19970529
	NO 9805711	A	19981207	NO 1998-5711	19981207
PRAI	US 1996-655912	A	19960531		
	US 1996-656063	A	19960531		
	US 1997-808754	A	19970227		
	US 1997-808755	A	19970227		
	US 1997-807682	A	19970227		
	WO 1997-US9450	W	19970529		

OS MARPAT 128:48490
AB Amino acid derivs. R2RxRyXR1NR3(R3*)nCR4R4*R5 [X = N, C (R2 not present when X = N); R2 = H, alkyl, alkoxy, cyano, alkanoyl, etc.; Rx, Ry = aryl, heteroaryl, adamantyl, or nonarom. ring linked to X via a single bond, alkylene, etc.; R1 = alkylene, iminooxyethylene, etc.; R3 = H, alkyl, (un)substituted Ph or phenylalkyl, etc.; R3* = alkyl, O; n = 0, 1; R4, R4* = H, alkyl, hydroxyalkyl; R5 = (un)substituted carbamoyl, carboxy, aminosulfonyl, phosphoryl, etc.] were prepd. as pharmaceuticals for treatment of neurol. and neuropsychiatric disorders. Thus, N-(4,4-diphenyl-3-butenyl)glycine Et ester was by alkylation of glycine Et ester hydrochloride with 4-bromo-1,1-diphenyl-1-butene. Binding assays to measure interaction of compds. with the glycine site on the NMDA receptor are illustrated.
IT **200004-42-8P 200004-51-9P 200004-53-1P**
200004-54-2P 200004-56-4P 200004-58-6P
200004-59-7P 200004-66-6P 200004-67-7P
200004-70-2P 200004-71-3P 200004-73-5P

200004-75-7P 200004-76-8P 200004-77-9P
200004-78-0P 200004-79-1P 200004-80-4P
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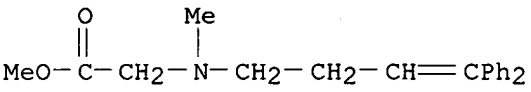
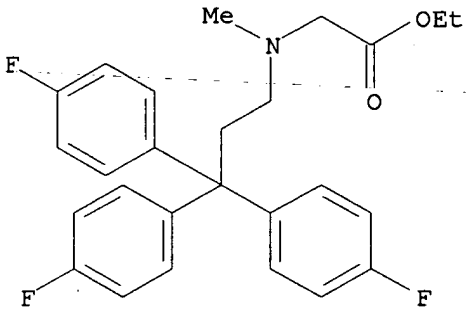
200005-34-1P 200005-46-5P 200005-51-2P
200005-52-3P 200005-54-5P 200006-07-1P
200006-08-2P 200006-09-3P 200006-10-6P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid derivs. as pharmaceuticals for treatment of neurol. and neuropsychiatric disorders)

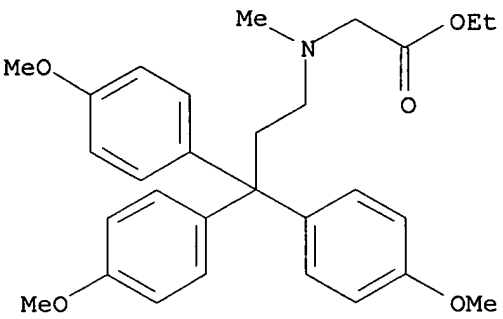
RN 200004-42-8 HCAPLUS
CN Glycine, N-(4,4-diphenyl-3-butenyl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

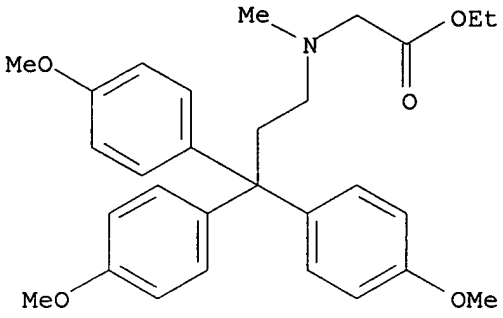


RN 200004-51-9 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-fluorophenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

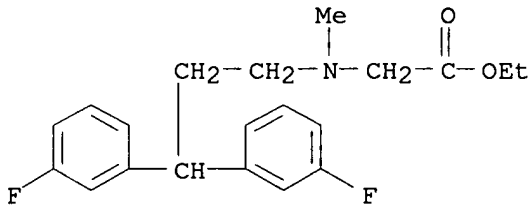


RN 200004-53-1 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-methoxyphenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

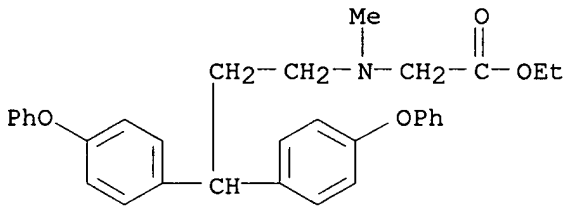




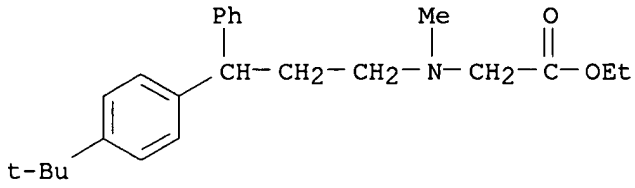
RN 200004-54-2 HCAPLUS
CN Glycine, N-[3,3-bis(3-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



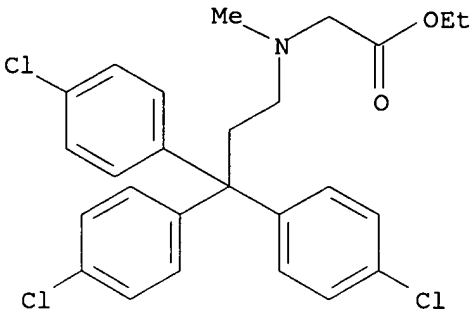
RN 200004-56-4 HCAPLUS
CN Glycine, N-[3,3-bis(4-phenoxyphenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



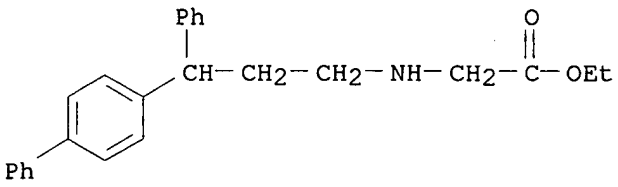
RN 200004-58-6 HCAPLUS
CN Glycine, N-[3-[4-(1,1-dimethylethyl)phenyl]-3-phenylpropyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



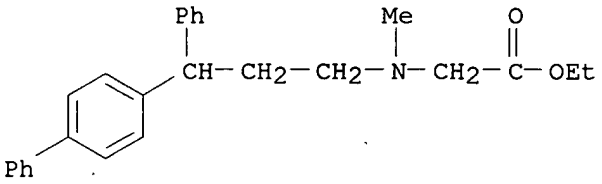
RN 200004-59-7 HCAPLUS
CN Glycine, N-methyl-N-[3,3,3-tris(4-chlorophenyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)



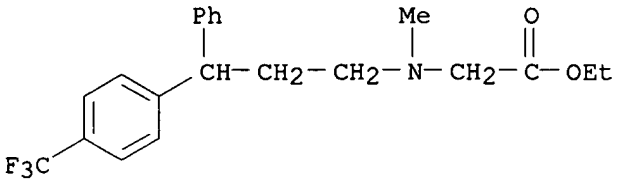
RN 200004-66-6 HCAPLUS
CN Glycine, N-(3-[1,1'-biphenyl]-4-yl-3-phenylpropyl)-, ethyl ester (9CI) (CA INDEX NAME)



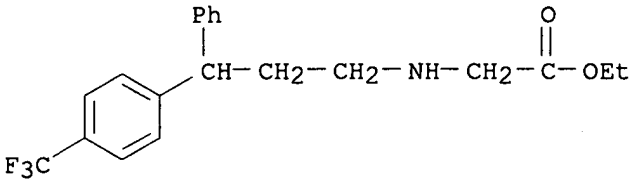
RN 200004-67-7 HCAPLUS
CN Glycine, N-(3-[1,1'-biphenyl]-4-yl-3-phenylpropyl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



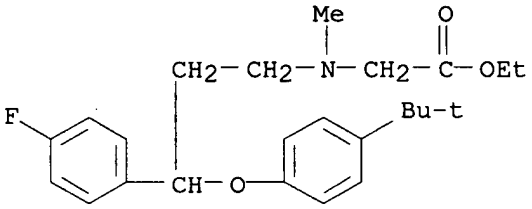
RN 200004-70-2 HCAPLUS
CN Glycine, N-methyl-N-[3-phenyl-3-[4-(trifluoromethyl)phenyl]propyl]-, ethyl ester (9CI) (CA INDEX NAME)



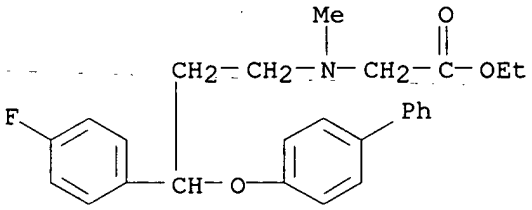
RN 200004-71-3 HCAPLUS
CN Glycine, N-[3-phenyl-3-[4-(trifluoromethyl)phenyl]propyl]-, ethyl ester (9CI) (CA INDEX NAME)



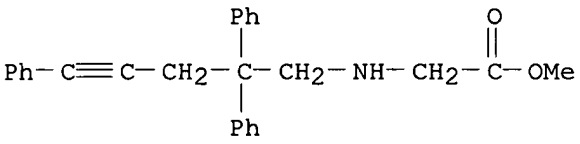
RN 200004-73-5 HCAPLUS
CN Glycine, N-[3-[4-(1,1-dimethylethyl)phenoxy]-3-(4-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 200004-75-7 HCAPLUS
CN Glycine, N-[3-([1,1'-biphenyl]-4-yloxy)-3-(4-fluorophenyl)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



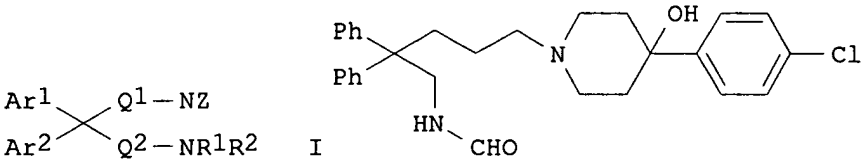
L28 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1997:749973 HCAPLUS
DN 128:75259
TI A thermal bicyclization. Synthesis of substituted 2,3,5,6-tetrahydro-6-oxo-1H-pyrrolizines
AU Belotti, D.; Cossy, J.
CS Laboratoire Chimie Organique, ESPCI, Paris, F-75231, Fr.
SO Synlett (1997), (11), 1249-1250
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 128:75259
AB 2,3,5,6-Tetrahydro-6-oxo-1H-pyrrolizines, potential precursors of 2,3-dihydro-1H-pyrrolizines were synthesized by a smooth, thermal, acid-promoted bicyclization of N-.omega.-acetylenic amino esters.
IT **200557-08-0**
RL: RCT (Reactant)
(prepn. of hydropyrrolizinones by thermal bicyclization)
RN 200557-08-0 HCAPLUS
CN Glycine, N-(2,2,5-triphenyl-4-pentynyl)-, methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1997:543479 HCAPLUS
DN 127:161698
TI Heterocyclic diphenylmethane derivatives as MIP-1.alpha./RANTES receptor antagonists
IN Kato, Kaneyoshi; Yamamoto, Mitsuo; Honda, Susumu; Fujisawa, Tomoyuki
PA Takeda Chemical Industries, Ltd., Japan; Kato, Kaneyoshi; Yamamoto, Mitsuo; Honda, Susumu; Fujisawa, Tomoyuki
SO PCT Int. Appl., 250 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9724325	A1	19970710	WO 1996-JP3820	19961226
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9712083	A1	19970728	AU 1997-12083	19961226

JP 10081665 A2 19980331 JP 1996-349136 19961227
PRAI JP 1995-343905 19951228
JP 1996-187375 19960717
WO 1996-JP3820 19961226
OS MARPAT 127:161698
GI

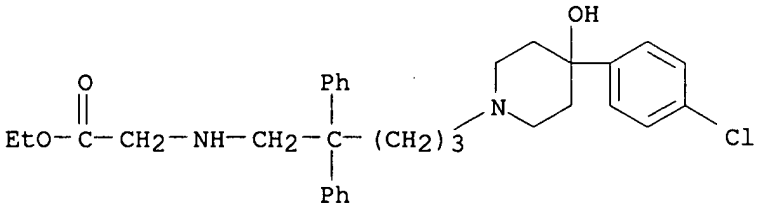


AB Compds. which are MIP-1.alpha./RANTES-receptor antagonists are disclosed, specifically I [Ar1, Ar2 = (un)substituted arom. group; Q1, Q2 = (un)substituted divalent C1-6 aliph. hydrocarbon group which may have either O or S within the C chain; R1 = H, (un)substituted alkyl or (un)substituted alkylcarbonyl; R2 = (un)substituted hydrocarbon group or (un)substituted acyl; or NR1R2 = (un)substituted N-contg. heterocyclic; NZ = (un)substituted N-contg. mono- or fused heterocyclic group], and salts thereof. The compds. are useful for therapy or prophylaxis of inflammatory, allergic, and other diseases. Over 120 title compds., and a variety of intermediates, were prepd. For instance, N-alkylation of 4-(4-chlorophenyl)-4-hydroxypiperidine by 5-(formylamino)-1-iodo-4,4-diphenylpentane in MeCN in the presence of K2CO3 at 60.degree. gave title compd. II, isolated as the monohydrochloride (III). III displaced 125I-RANTES from human RANTES receptors in vitro with an IC50 of 0.04 .mu.M, vs. 3 .mu.M for ioperamide.

IT **193541-61-6P 193541-62-7P 193541-63-8P 193541-64-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic diphenylmethane derivs. as MIP-1.alpha./RANTES receptor antagonists)

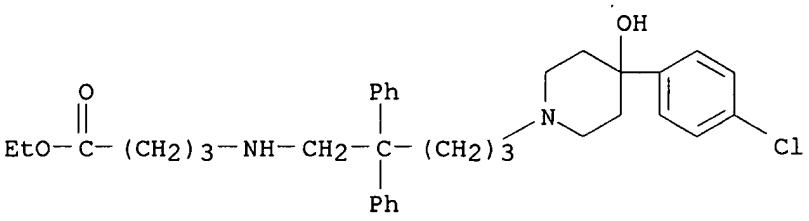
RN 193541-61-6 HCAPLUS

CN Glycine, N-[5-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-2,2-diphenylpentyl]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)



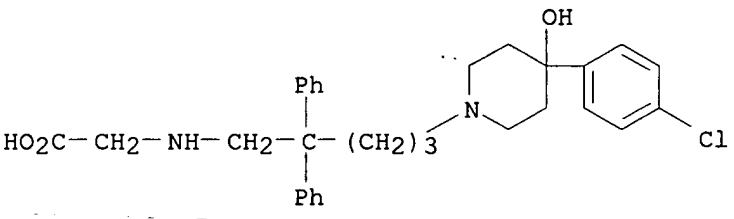
2 HCl

RN 193541-62-7 HCAPLUS
CN Butanoic acid, 4-[[5-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-2,2-diphenylpentyl]amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

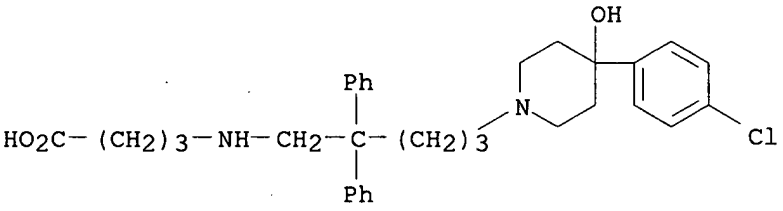


●2 HCl

RN 193541-63-8 HCAPLUS
CN Glycine, N-[5-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-2,2-diphenylpentyl]- (9CI) (CA INDEX NAME)



RN 193541-64-9 HCAPLUS
CN Butanoic acid, 4-[[5-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-2,2-diphenylpentyl]amino]- (9CI) (CA INDEX NAME)



L28 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1997:473595 HCAPLUS
DN 127:81788
TI Preparation of amino acid derivatives as neuropeptide Y antagonists
IN Engel, Wolfhard; Eberlein, Wolfgang; Rudolf, Klaus; Doods, Henri; Wieland, Heike-Andrea; Willim, Klaus-Dieter; Entzeroth, Michael; Wienen, Wolfgang
PA Dr. Karl Thomae Gmbh, Germany
SO Ger. Offen., 117 pp.
CODEN: GWXXBX

DT Patent
LA German
FAN.CNT 1

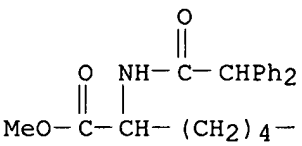
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19544687	A1	19970605	DE 1995-19544687	19951130
	WO 9719911	A1	19970605	WO 1996-EP5222	19961126
	W: CA, JP, MX, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 885186	A1	19981223	EP 1996-941032	19961126
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2000501390	T2	20000208	JP 1997-520166	19961126
	US 6114390	A	20000905	US 1997-950113	19971014
PRAI	DE 1995-19544687	A	19951130		
	WO 1996-EP5222	W	19961126		
	US 1998-945048	A	19980210		

OS MARPAT 127:81788

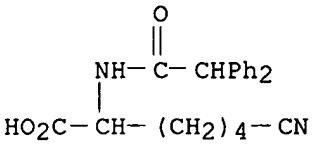
AB Title compds. T-Z-CONHCH(CH2B)CO-Y-(CH2)nR [I; T = (un)substituted Ph, naphthyl, heteroarom., N, O, S, or T1TC2U; T1, T2 = (un)substituted Ph; U = H, alkoxy, OPh; Z = bond, O, NH, CH2, CH2CH2, CH2O, CH2NH; B = amidine-contg. group; Y = O, NR1; R1 = H, (un)substituted alkyl, CH2Ph; n = 1-3; R = (un)substituted Ph], neuropeptide Y antagonists, were prepd. Thus, (R)-R2NHC(:NH)NH(CH2)3CH(NHR3)CONHR4 [II; R2 = 2,2,5,7,8-pentamethylchroman-6-sulfonyl (Pmc); R3, = Fmoc; R4 = CH2C6H4CH2NHCO2CH2Ph-4] was prepd. from Fmoc-D-Arg(Pmc)OH and 4-PhCH2O2CNHCH2C6H4CH2CONH2, Fmoc-deprotected, and diphenylacetylated, to give II (R2 = Pmc; R3 = COCHPh2; R4 = CH2C6H4CH2NH2-4), which was N-acetylated and deprotected to give II-trifluoroacetate (R2 = H; R3 = COCHPh2; R4 = CH2C6H4CH2NHAc-4). I showed activity as neuropeptide Y antagonists in both in vitro (at 10-8 to 10-5 M) and in vivo tests (at 0.001 to 10 mg/kg).

IT **191871-83-7P 191871-84-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of amino acid derivs. as neuropeptide Y antagonists)

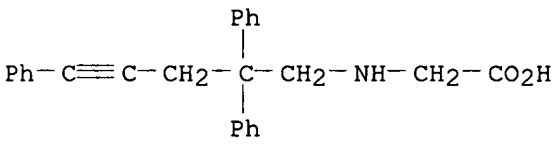
RN 191871-83-7 HCAPLUS
CN Hexanoic acid, 6-cyano-2-[(diphenylacetyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 191871-84-8 HCAPLUS
CN Hexanoic acid, 6-cyano-2-[(diphenylacetyl)amino]- (9CI) (CA INDEX NAME)



L28 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1997:269718 HCAPLUS
DN 127:4979
TI Cyclization of .delta.,.epsilon.-acetylenic amines and amino acids into cyclic enamines. A very efficient and simple access to polysubstituted pyrrolidines
AU Cossy, J.; Belotti, D.; Bellosta, V.; Boggio, C.
CS Laboratoire de Chimie Organique, Associe au CNRS, ESPCI, Paris, 75231, Fr.
SO Tetrahedron Lett. (1997), 38(15), 2677-2680
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
AB The thermolysis of .delta.,.epsilon.-acetylenic amines and amino acids led to cyclic enamines which after redn. with NaBH(OAc)3 were transformed into polysubstituted pyrrolidines.
IT **190261-42-8**
RL: RCT (Reactant)
(cyclization of .delta.,.epsilon.-acetylenic amines and amino acids into cyclic enamines)
RN 190261-42-8 HCAPLUS
CN Glycine, N-(2,2,5-triphenyl-4-pentynyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1996:740277 HCAPLUS
DN 126:7822
TI Methadone derivatives and protein and polypeptide methadone derivative conjugates and labels
IN Buechler, Kenneth F.
PA Biosite Diagnostics, Incorporated, USA
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9631496	A1	19961010	WO 1996-US2560	19960308
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML				
	US 5710256	A	19980120	US 1995-416034	19950403
	CA 2217154	AA	19961010	CA 1996-2217154	19960308
	AU 9651739	A1	19961023	AU 1996-51739	19960308

	EP 827502	A1	19980311	EP 1996-908525	19960308
	EP 827502	B1	20001122		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 11503428	T2	19990326	JP 1996-530280	19960308
	AT 197709	E	20001215	AT 1996-908525	19960308
PRAI	US 1995-416034	A	19950403		
	WO 1996-US2560	W	19960308		

OS MARPAT 126:7822

AB Methadone derivs. are synthesized and covalently attached to antigens (proteins or polypeptides) in order to prep. antibodies or receptors to methadone and methadone metabolites. Once generated, the antibodies or receptors and the derivs. which are covalently attached to proteins, polypeptides or labels may be used in the immunoassay process (no data). In the single example given, 1-N-cysteinamido-6,6-diphenyl-5-keto-8-(dimethylamino)nonane was prepd. in several steps from 2,2-diphenyl-4-(dimethylamino)pentanenitrile.

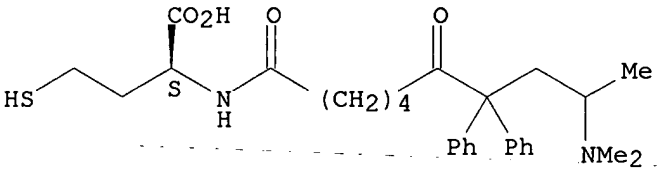
IT **184093-39-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of methadone derivs.)

RN 184093-39-8 HCAPLUS

CN L-Homocysteine, N-[9-(dimethylamino)-1,6-dioxo-7,7-diphenyldecyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

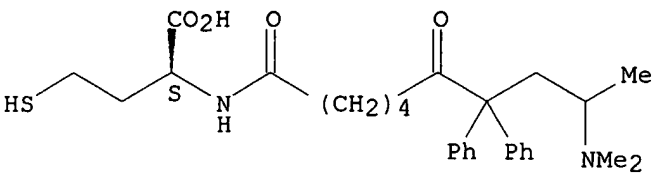
IT **184093-38-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of methadone derivs.)

RN 184093-38-7 HCAPLUS

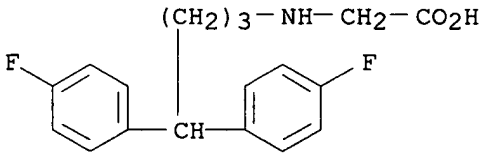
CN L-Homocysteine, N-[9-(dimethylamino)-1,6-dioxo-7,7-diphenyldecyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2002 ACS

AN 1995:889841 HCAPLUS
DN 124:118
TI Identification of amperozide metabolites in urine from rats, rabbits, dogs and man by Frit-FAB LC/MS using deuterated solvents to gain additional structural information
AU Edlund, P. O.
CS Dep. Structural Biochem., Biopharmaceuticals, Stockholm, S-11287, Swed.
SO J. Mass Spectrom. (1995), 30(10), 1380-92
CODEN: JMSPFJ; ISSN: 1076-5174
DT Journal
LA English
AB A general procedure for screening of amperozide, N-ethyl-4-[4,4-bis(p-fluorophenylbutyl)]-1-piperazine carboxamide, labeled with 3H and 14C was developed. Urine exts. were first fractionated by preparative reversed phase chromatog. with an acetonitrile gradient elution. The collected fractions, were finally analyzed using a methanol gradient on packed capillary LC columns with an internal diam. of 0.32 or 0.5 mm connected to the Frit-FAB probe of a Jeol SX-102 mass spectrometer for structural anal. A micro-gradient system dedicated for the use of deuterated solvents was constructed from two six-port switching valves to reduce the consumption of the eluents. The no. of hydrogens bound to heteroatoms (OH, NH) was detd. by comparing the spectra recorded from mobile phases using water and deuterium oxide. The mass spectra recorded during elution with deuterated solvents was also useful for the interpretation of the fragmentation pattern of std. compds. and unknown metabolites. The technique proved esp. useful of different between hydroxylation and N-oxidn. which gave the same increase in mol. mass by 16 u but a difference in the no. of exchangeable protons. Metabolites formed by oxidative N-dealkylation of amperozide either at the basic nitrogen or a the N-ethylcarboxamide nitrogen were identified. Addnl. metabolites derived from deethylated amperozide involving N-oxidn. of the basic nitrogen of the piperazine ring and/or hydroxylation of the piperazine ring were identified. Metabolites formed by oxidative N-dealkylation and opening of the piperazine ring were also identified.
IT **171202-47-4**
RL: ANT (Analyte); ANST (Analytical study)
(identification of amperozide metabolites in urine from rats, rabbits, dogs and man by Frit-FAB LC/MS)
RN 171202-47-4 HCAPLUS
CN Glycine, N-[4,4-bis(4-fluorophenyl)butyl]- (9CI) (CA INDEX NAME)



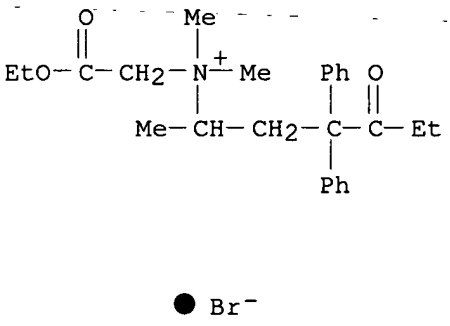
L28 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:887981 HCAPLUS
DN 123:275962
TI Quaternary ammonium immunogenic conjugates and immunoassay reagent.
IN Craig, Alan R.
PA du Pont de Nemours, E. I., and Co., USA
SO Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

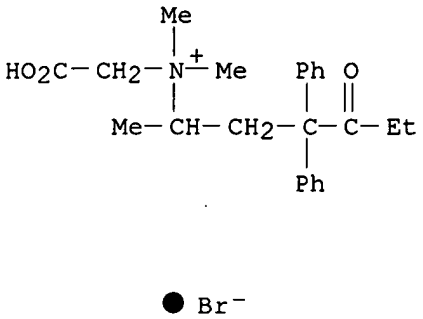
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 668504	A1	19950823	EP 1995-101210	19950130
	EP 668504	B1	20010321		
	R: DE, FR, IT				
	US 5492841	A	19960220	US 1994-199380	19940218
	JP 07260784	A2	19951013	JP 1995-29300	19950217
	JP 2731739	B2	19980325		
PRAI	US 1994-199380	A	19940218		

AB This invention relates to novel quaternary immunogenic conjugates and reporter reagents useful for eliciting antibodies and in immunoassays. The hapten of the quaternary ammonium conjugate is selected from the group consisting of cocaine, methadone, methaqualone, propoxyphene, phencyclidine, amphetamine, benzodiazepam, quinidine, procainamide, N-acetylprocainamide, and tricyclic amines. The carrier for the conjugate is selected from the group consisting of proteins, glycoproteins, polypeptides, carbohydrates, and latex particles. Processes for prepg. such quaternary ammonium immunogenic conjugates and their use in immunoassays and in eliciting antibodies are also disclosed.

IT **169552-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of quaternary ammonium immunogenic conjugates of methadone)
RN 169552-88-9 HCAPLUS
CN Benzenepropanaminium, N-(2-ethoxy-2-oxoethyl)-N,N,.alpha.-trimethyl-.gamma.-(1-oxopropyl)-.gamma.-phenyl-, bromide (9CI) (CA INDEX NAME)



IT **169552-89-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of quaternary ammonium immunogenic conjugates of methadone)
RN 169552-89-0 HCAPLUS
CN Benzenepropanaminium, N-(carboxymethyl)-N,N,.alpha.-trimethyl-.gamma.-(1-oxopropyl)-.gamma.-phenyl-, bromide (9CI) (CA INDEX NAME)



L28 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:723199 HCAPLUS
DN 123:143931
TI Preparation of condensed seven-membered heterocyclic compounds useful as squalene synthetase inhibitors
IN Yukimasa, Hidefumi; Tozawa, Ryuichi; Sugiyama, Yasuo; Kori, Masakuni
PA Takeda Chemical Industries, Ltd., Japan
SO Eur. Pat. Appl., 98 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 2

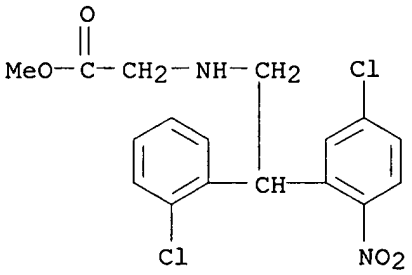
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 645378	A1	19950329	EP 1994-114837	19940921
	EP 645378	B1	20000823		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	AU 9473051	A1	19950406	AU 1994-73051	19940916
	AU 678503	B2	19970529		
	NO 9403495	A	19950327	NO 1994-3495	19940920
	AT 195732	E	20000915	AT 1994-114837	19940921
	AT 156820	E	19970815	AT 1994-114939	19940922
	CA 2132792	AA	19950325	CA 1994-2132792	19940923
	CA 2132794	AA	19950325	CA 1994-2132794	19940923
	FI 9404418	A	19950325	FI 1994-4418	19940923
	HU 70962	A2	19951128	HU 1994-2739	19940923
	RU 2129547	C1	19990427	RU 1994-34115	19940923
	CN 1106397	A	19950809	CN 1994-116486	19940924
	CN 1054380	B	20000712		
	JP 07179444	A2	19950718	JP 1994-229159	19940926
	JP 07179429	A2	19950718	JP 1994-229160	19940926
	US 5698691	A	19971216	US 1994-311932	19940926
	US 5677298	A	19971014	US 1996-696118	19960813
PRAI	JP 1993-238273	A	19930924		
	JP 1993-241062	A	19930928		
	US 1994-312194	B1	19940926		

OS MARPAT 123:143931
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; A = (un)substituted benzo or heterocyclo moiety; D, K = C, N; R1 = H, (un)substituted hydrocarbyl; R2 = H, (un)substituted alkyl, (un)substituted Ph, (un)substituted arom. heterocyclyl; X = esterified carboxyl, (un)substituted carbamoyl, (un)substituted OH,

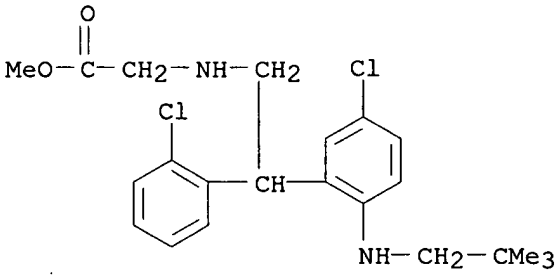
(un)substituted NH2, (un)substituted heterocyclyl; Z = C, N, S(O)q; q = 0-2; ring J is an (un)substituted 7-membered heterocyclic ring contg. .ltoreq.3 heteroatoms], useful as inhibitors of squalene synthetase which do not inhibit the biosynthesis of ubiquinone (no data), heme A (no data), or dolichol (no data), and which are useful in the treatment of hypercholesteremia (no data) or coronary sclerosis (no data), are prepd. and I-contg. formulations presented. Thus, benzothiazepinone, II, was prepd. and demonstrated a IC50 against human squalene synthetase of 0.10 x 10-7 M.

IT **165952-41-0P 165952-45-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of condensed seven-membered heterocyclic compds. useful as squalene synthetase inhibitors from)

RN 165952-41-0 HCAPLUS
CN Glycine, N-[2-(5-chloro-2-nitrophenyl)-2-(2-chlorophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 165952-45-4 HCAPLUS
CN Glycine, N-[2-[5-chloro-2-[(2,2-dimethylpropyl)amino]phenyl]-2-(2-chlorophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:662328 HCAPLUS
DN 123:83996
TI Preparation of aminoacid derivatives as neuropeptide Y antagonists.
IN Rudolf, Klaus; Eberlein, Wolfgang; Engel, Wolfhard; Mihm, Gerhard; Doods, Henri; Wieland, Heike-Andrea; Willim, Klaus-Dieter; Krause, Juergen; Dollinger, Horst; et al.
PA Dr. Karl Thomae GmbH, Germany
SO PCT Int. Appl., 308 pp.

CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9417035	A1	19940804	WO 1994-EP109	19940118
	W: AU, BG, BY, CA, CN, CZ, FI, HU, JP, KR, NO, NZ, PL, RO, RU, SK, UA				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 4301452	A1	19940721	DE 1993-4301452	19930120
	DE 4326465	A1	19950209	DE 1993-4326465	19930806
	AU 9458841	A1	19940815	AU 1994-58841	19940118
	AU 683442	B2	19971113		
	EP 680469	A1	19951108	EP 1994-905073	19940118
	EP 680469	B1	20000426		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08505862	T2	19960625	JP 1994-516636	19940118
	AT 192142	E	20000515	AT 1994-905073	19940118
	FI 9503467	A	19950718	FI 1995-3467	19950718
	NO 9502869	A	19950919	NO 1995-2869	19950719
PRAI	DE 1993-4301452	A	19930120		
	DE 1993-4326465	A	19930806		
	WO 1994-EP109	W	19940118		

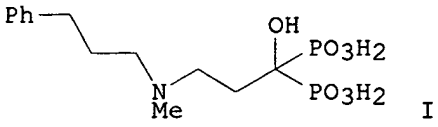
OS MARPAT 123:83996
AB TZNR1CR2R3COY(CH2)nR [n = 0-5; R = H, OH, (substituted) Ph, naphthyl, aminophenyl, aminonaphthyl, hydroxyphenyl, hydroxynaphthyl, diphenylmethyl, heteroaryl, cycloalkyl, etc.; Y = O, NR4; R1, R4 = H, alkyl, cycloalkyl, (substituted) Ph, PhCH2; R2 = substituted alkyl, Ph, PhCH2; R3 = H, alkyl, cycloalkyl; T = H, Ph, (substituted) heteroaryl, protecting group, etc.; Z = bond, CO, CH2, SO, SO2], were prepd. Thus, H-D-Arg(NO2)-OH in THF was treated with aq. NaOH and then with Ph2CHCOCl to give 85% amide. This in THF was treated with N-methylmorpholine, iso-Bu chloroformate, and 4-(aminomethyl)acetanilide under cooling to give 63% (R)-N-[[4-(acetylamino)phenyl]methyl]-N5-[amino(nitroimino)methyl]-N2-(diphenylacetyl)ornithinamide. This was hydrogenated in aq. HOAc over Pd to give (R)-N-[[4-(acetylamino)phenyl]methyl]-N2-diphenylacetylargininamide acetate. Title compds. antagonized neuropeptide Y-induced effects on blood pressure in rats at 0.01-10 mg/kg.
IT **164648-22-0P 164648-23-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aminoacid derivs. as neuropeptide Y antagonists)
RN 164648-22-0 HCAPLUS
RN 164648-23-1 HCAPLUS

L28 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1992:511804 HCAPLUS
DN 117:111804
TI Preparation of (araliphatylamino)alkanediphosphonic acids as calcium metabolism regulators
IN Jaeggi, Knut A.
PA Ciba-Geigy Corp., USA
SO U.S., 11 pp. Cont.-in-part of U.S. Ser. No. 278,394, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	US 5110807	A	19920505	US 1990-500441	19900328
	US 5190930	A	19930302	US 1991-811590	19911220
PRAI	US 1988-278394		19881201		
	CH 1987-4847		19871211		
	US 1990-500441		19900328		
OS	MARPAT 117:111804				

GI



I

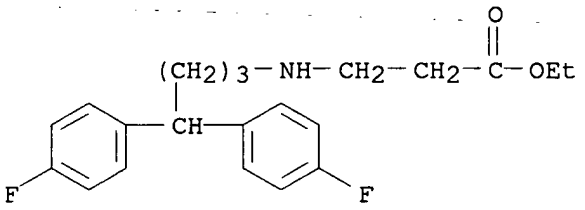
AB R1R2NX C(OH)(PO3H2)2 (R1 = araliphatyl; R2 = H, monovalent aliphatyl; X = divalent aliphatyl), were prepd. for treatment of Ca metab. disorders (no data). Thus, 3-[N-(3-phenylpropyl)-N-methylamino]propionic acid-HCl (prepn. given) was heated at 100.degree. with 85% H3PO4, PhCl, and PCl3 to give a residue which was refluxed with 9N HCl to give title compd. I. Tablets were prepd. contg. I.

IT **124369-91-1P 143070-50-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate of calcium regulator)

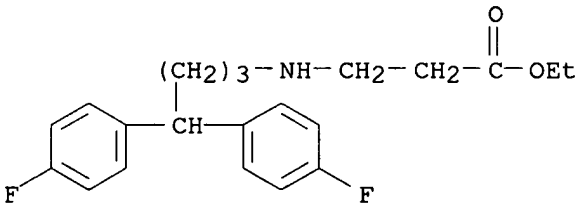
RN 124369-91-1 HCAPLUS

CN .beta.-Alanine, N-[4,4-bis(4-fluorophenyl)butyl]-, ethyl ester (9CI) (CA INDEX NAME)



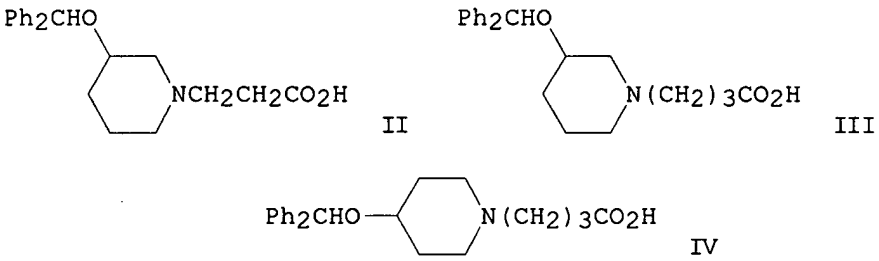
RN 143070-50-2 HCAPLUS

CN .beta.-Alanine, N-[4,4-bis(4-fluorophenyl)butyl]-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



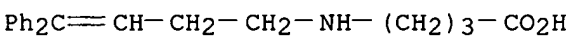
HCl

L28 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1991:247711 HCAPLUS
DN 114:247711
TI GABA uptake inhibitors. Syntheses and structure-activity studies on GABA analogs containing diarylbutenyl and diarylmethoxyalkyl N-substituents
AU Falch, E.; Krogsgaard-Larsen, P.
CS Dep. Org. Chem., R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.
SO Eur. J. Med. Chem. (1991), 26(1), 69-77
CODEN: EJMCA5; ISSN: 0223-5234
DT Journal
LA English
OS CASREACT 114:247711
GI



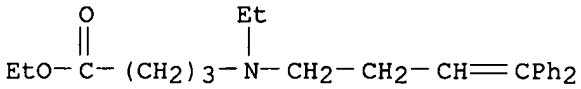
AB A no. of analogs of GABA or .beta.-alanine contg. 4,4-diphenyl-3-butenyl (DPB), benzhydryl Et ether (BEE), or benzhydryl Pr ether N-substituents have been synthesized and tested as inhibitors of synaptosomal GABA uptake. Whereas the N-DPB and N-BEE analogs of GABA are markedly less potent than GABA itself as inhibitors of GABA uptake, N-methylation of these analogs resulted in increased potency and reduced pKa II values of Ph2C:CHCH2NMe(CH2)3CO2H and Ph2CHOCH2CH2NMe(CH2)3CO2H (I). Incorporation of the alkyl groups of Ph2CHOCH2CH2NMeCH2CH2CO2H, I, and Ph2CHO(CH2)3NMe(CH2)3CO2H into the cyclized piperidine analogs gave the less active compds. II, III, and IV, resp. This loss of in vitro activity was most pronounced for III and IV. These results suggest that the basic chatacter of the amino groups as well as the conformational flexibility of the spacer-arm connecting the amino acid 'heads' and the arom. moieties of this class of GABA uptake inhibitors are factors of importance for GABA uptake affinity.

IT **95274-11-6**
RL: RCT (Reactant)
(inhibition by, of synaptosomal GABA uptake)
RN 95274-11-6 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)amino]- (9CI) (CA INDEX NAME)

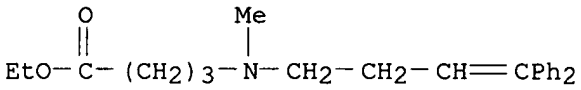


IT **133992-88-8P 134014-86-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
RN 133992-88-8 HCAPLUS

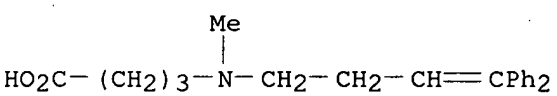
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)ethylamino]-, ethyl ester (9CI) (CA INDEX NAME)



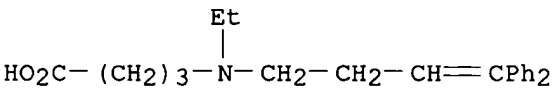
RN 134014-86-1 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



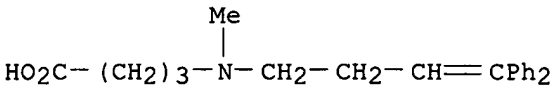
IT **133992-89-9P 133992-90-2P 133993-13-2P 133993-14-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and synaptosomal GABA uptake-inhibiting activity of)
RN 133992-89-9 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)methylamino]-, hydrochloride (9CI) (CA INDEX NAME)



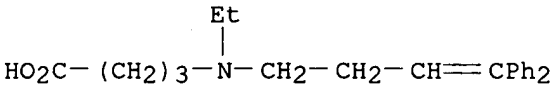
RN 133992-90-2 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)ethylamino]-, hydrochloride (9CI) (CA INDEX NAME)



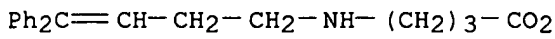
RN 133993-13-2 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)methylamino]- (9CI) (CA INDEX NAME)



RN 133993-14-3 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)ethylamino]- (9CI) (CA INDEX NAME)



L28 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1991:74729 HCAPLUS
DN 114:74729
TI GABA-A agonists and GABA uptake inhibitors: structure-activity relationships
AU Falch, Erik; Larsson, Orla M.; Schousboe, Arne; Krogsgaard-Larsen, Povl
CS Dep. Org. Chem., R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.
SO Drug Dev. Res. (1990), 21(3), 169-88
CODEN: DDREDK; ISSN: 0272-4391
DT Journal
LA English
AB Muscimol is a potent but non-selective GABA-A agonist. Structure-activity studies on the (S)- and (R)-forms of chiral muscimol analogs have disclosed a high degree of agonist stereoselectivity of the GABA-A receptors. THIP (4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridin-3-ol) is a specific GABA-A agonist which has been the subject of clin. studies in different groups of patients. Even minor alterations of the structure of THIP result in substantial or complete loss of GABA-A agonist activity. 4-PIOL (5-(4-piperidyl)isoxazol-3-ol) shows in vivo GABA-A agonist activity on spinal neurons, whereas the in vitro pharmacol. effects in brain tissue prepns. are consistent with a GABA-A antagonist profile of 4-PIOL in the brain. Whereas nipetcotic acid and related GABA uptake inhibitors are substrates for the neuronal and glial transport carriers, the glia-selective GABA uptake inhibitors THPO (4,5,6,7-tetrahydroisoxazolo[4,5-c]pyridin-3-ol) and probably also THAO (5,6,7,8-tetrahydro-4H-isoxazolo[4,5-c]azepin-3-ol) are not being transported by the glial uptake carrier. Introduction of the DPB (4,4-diphenyl-3-butenyl) or BEE (benzhydryl Et ether) substituents on the basic atoms of GABA uptake inhibitors including nipecotic acid and THPO, results in markedly more potent inhibitors. However, unlike THPO, N-DPB-THPO interacts non-selectively with neuronal and glial GABA uptake, and, in contrast to nipecotic acid, N-DPB-nipecotic acid (SKF-89976-A) has been shown not to be transported by the neuronal or glial GABA carriers. Whereas N-DPB- and N-BEE-GABA are weak inhibitors of synaptosomal GABA uptake, N-methylation of these compds. gives potent uptake inhibitors.
IT **95274-11-6**
RL: BIOL (Biological study)
(as GABA uptake inhibitor, structure in relation to)
RN 95274-11-6 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)amino]- (9CI) (CA INDEX NAME)



L28 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1990:48261 HCAPLUS
DN 112:48261
TI GABA uptake inhibitors containing mono- and diarylmethoxyalkyl N-substituents
AU Falch, Erik; Krogsgaard-Larsen, Povl
CS PharmaBiotec Res. Cent., R. Dan. Sch. Pharm., Copenhagen, DK-2100, Den.
SO Drug Des. Delivery (1989), 4(3), 205-15
CODEN: DDDEEJ; ISSN: 0884-2884
DT Journal
LA English
AB Analogs of GABA and the GABA uptake inhibitors, nipecotic acid and guvacine, carrying N-(mono)- or N-(diarylmethoxy)alkyl substituents were synthesized and tested in vitro as inhibitors of synaptosomal GABA uptake and GABAA receptor binding. Whereas the N-(diphenylmethoxy)ethyl deriv. of GABA was only a moderately potent inhibitor of GABA uptake, corresponding derivs. of nipecotic acid (I) and guvacine were potent inhibitors having IC50 values in the low micromolar range. In the case of I the (R)-isomer was 3 times more potent than the (S)-isomer, the bis-4-chlorophenyl analog was more potent than I, the introduction of an addnl. methylene group into the linkage between the nipecotic acid and benzhydryl ether moiety did not affect the in vitro biol. activity, and removal of one of the Ph groups, or replacement of the benzhydryl ether group by the conformationally restrained fluorenyloxy group resulted in a substantial loss of activity. None of the compds. synthesized showed detectable affinity for GABAA receptor sites.
IT **95274-11-6**
RL: BIOL (Biological study)
(GABA uptake inhibition by, structure in relation to)
RN 95274-11-6 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)amino]- (9CI) (CA INDEX NAME)

L28 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1990:21139 HCAPLUS
DN 112:21139
TI Preparation and formulation of araliphatyl aminoalkyldiphosphonic acids for treatment of disorders of calcium metabolism
IN Jaeggi, Knut A.
PA Ciba-Geigy A.-G., Switz.
SO Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 320455	A1	19890614	EP 1988-810830	19881202

	EP 320455	B1	19930609			
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
	AT 90353	E	19930615	AT	1988-810830	19881202
	ES 2054868	T3	19940816	ES	1988-810830	19881202
	ZA 8809157	A	19890726	ZA	1988-9157	19881207
	IL 88620	A1	19941128	IL	1988-88620	19881207
	JP 01197495	A2	19890809	JP	1988-308986	19881208
	DK 8806884	A	19890612	DK	1988-6884	19881209
	FI 8805710	A	19890612	FI	1988-5710	19881209
	FI 92704	B	19940915			
	FI 92704	C	19941227			
	NO 8805489	A	19890612	NO	1988-5489	19881209
	NO 176663	B	19950130			
	NO 176663	C	19950510			
	AU 8826738	A1	19890615	AU	1988-26738	19881209
	AU 609549	B2	19910502			
	HU 48899	A2	19890728	HU	1988-6378	19881209
	HU 202880	B	19910429			
	DD 283631	A5	19901017	DD	1988-322931	19881209
	CA 1329609	A1	19940517	CA	1988-585416	19881209
PRAI	CH 1987-4847		19871211			
	EP 1988-810830		19881202			

OS MARPAT 112:21139

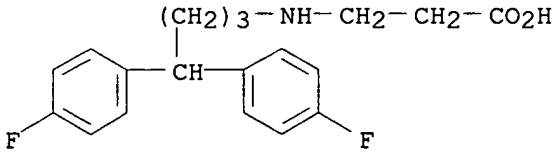
AB R1R2NXC(OH)(PO3H2)2 (I; R1 = arylaliph. residue; R2 = H, aliph. residue; X = divalent aliph. residue), useful for treating disturbances of Ca metab. (no data), were prepd. Thus, Ph(CH2)3NHMe in Et2O was treated with H2C:CHCO2Et and the mixt. was kept overnight to give Ph(CH2)3NMeCH2CH2CO2Et. The latter was hydrolyzed with HCl and the resulting carboxylic acid hydrochloride was stirred with 85% H3PO4 and PhCl at 100.degree. with addn. of PCl3. The mixt. was kept at 100.degree. for 3.5 h and the product was stirred for 3 h in refluxing 9 N HCl to give Ph(CH2)3NMeCH2CH2C(OH)(PO3H2)2 (II). Tablets were prepd. contg. II 75, lactose 268.5, cornstarch 22.5, polyethylene glycol 6000 5.0, talc 15.0, and Mg stearate 4.0 g/1000 tablets.

IT **124369-90-0P 124369-91-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for hydroxydiphosphonate calcium metab. regulator)

RN 124369-90-0 HCAPLUS

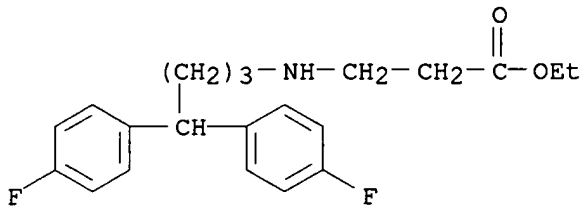
CN .beta.-Alanine, N-[4,4-bis(4-fluorophenyl)butyl]-, hydrochloride (9CI) (CA INDEX NAME)



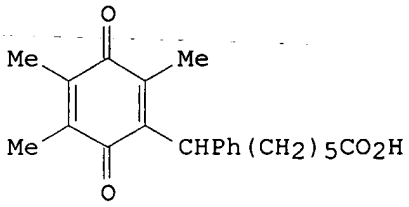
● HCl

RN 124369-91-1 HCAPLUS

CN .beta.-Alanine, N-[4,4-bis(4-fluorophenyl)butyl]-, ethyl ester (9CI) (CA INDEX NAME)



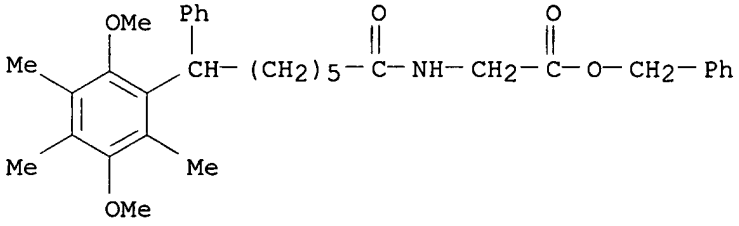
L28 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1989:514805 HCAPLUS
DN 111:114805
TI Quinones. 4. Novel eicosanoid antagonists: synthesis and pharmacological evaluation
AU Shiraishi, Mitsuru; Kato, Kaneyoshi; Terao, Shinji; Ashida, Yasuko; Terashita, Zenichi; Kito, Go
CS Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan
SO J. Med. Chem. (1989), 32(9), 2214-21
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 111:114805
GI



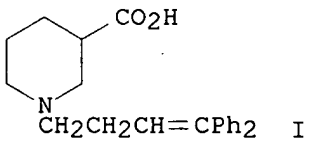
I

AB A series of .omega.-phenyl-.omega.-quinonylalkanoic acids and related compds. was synthesized. The compds. were tested for their inhibitory effects on U-44069-induced contraction of the rabbit aorta. (.+-.)-7-(3,5,6-Trimethyl-1,4-benzoquinon-2-yl)-7-phenylheptanoic acid (I) was one of the most potent compds. I inhibited U-46619-induced contraction of the guinea pig lung and U-44069-induced aggregation of the guinea pig platelet (ED50 = 3.5 .times. 10-7 M). I displaced [3H]U-46619 from guinea pig platelets (ED50 = 7.4 .times. 10-9 M). I also showed very potent inhibitory effects with a min. ED of 0.3 mg/kg orally on U-46619-, LTD4-, platelet activating factor-, or IgG1-induced bronchoconstriction in guinea pigs. The enantiomers of I were prepd. R-(+)-I was active in both in vitro and in vivo tests, but S-(-)-I was much less active. It is concluded that the antiasthmatic effects of I are due primarily to its antagonistic action on the TXA2 receptor. In addn., I showed potent inhibitory effects on PGD2-, PGF2.alpha.-, and 11-epi-PGF2a-induced contraction of guinea pig tracheal strips. The diverse inhibitory effects might be expressed in terms of eicosanoid-antagonistic activity.

IT **122115-66-6**
RL: RCT (Reactant)
(debenzylation of)
RN 122115-66-6 HCAPLUS
CN Glycine, N-[7-(2,5-dimethoxy-3,4,6-trimethylphenyl)-1-oxo-7-phenylheptyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



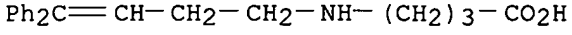
L28 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1985:160041 HCAPLUS
DN 102:160041
TI Orally active and potent inhibitors of .gamma.-aminobutyric acid uptake
AU Ali, Fadia E.; Bondinell, William E.; Dandridge, Penelope A.; Frazee, James S.; Garvey, Eleanor; Girard, Gerald R.; Kaiser, Carl; Ku, Thomas W.; Lafferty, John J.; et al.
CS Dep. Med. Chem., Smith Kline French Lab., Philadelphia, PA, 19101, USA
SO J. Med. Chem. (1985), 28(5), 653-60
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



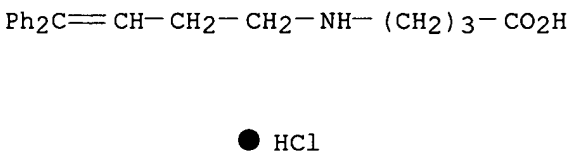
I

AB GABA [56-12-2]-uptake inhibitors that are more potent, more lipophilic, and in limited testing, at least as selective as the parent amino acids were obtained by alkylation of the appropriate butyric-, cyclohexane- and piperidinecarboxylic and pyrrolinidineacetic acids. The ability of these alkylated amino acids to inhibit Na-dependent, high-affinity GABA uptake was measured after preincubation for 15 min with rat brain synaptosomes. N-(4,4-Diphenyl-3-butenyl)-3-piperidinecarboxylic acid (I) [85375-85-5] is a specific GABA-uptake inhibitor more potent, more lipophilic and, as selective as the nonalkylated parent; I and its analogs also exhibited anticovulsant activity in rodents. Structure-activity relations are discussed.
IT **95274-11-6**

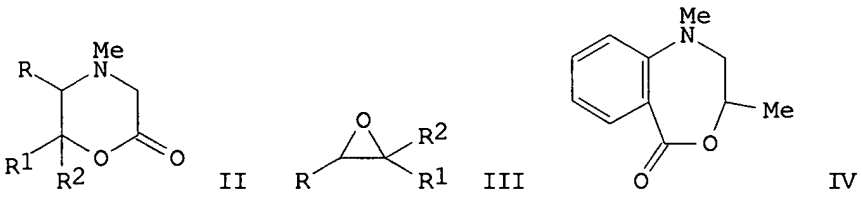
RL: BIOL (Biological study)
(GABA uptake inhibition by, in brain)
RN 95274-11-6 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)amino]- (9CI) (CA INDEX NAME)



IT **95274-10-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as GABA uptake inhibitor in brain)
RN 95274-10-5 HCAPLUS
CN Butanoic acid, 4-[(4,4-diphenyl-3-butenyl)amino]-, hydrochloride (9CI) (CA INDEX NAME)

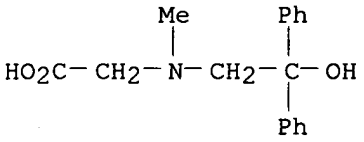


L28 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1983:215242 HCAPLUS
DN 98:215242
TI Lactones. II: Synthesis of dihydroxylated diphenylalkanamines via azalactones
AU Lehmann, Jochen
CS Pharm. Inst., Univ. Bonn, Bonn, 5300/1, Fed. Rep. Ger.
SO Arch. Pharm. (Weinheim, Ger.) (1983), 316(4), 339-46
CODEN: ARPMAS; ISSN: 0365-6233
DT Journal
LA German
GI

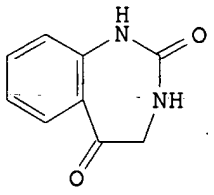


AB HOCPh2CH2NMeCHRCR1R2OH [I, R = H, Me; R1, R2 = H, Me, Ph; R1R2 = (CH2)4] were prepd. by treating morpholinones II with PhLi. II were prepd. by treating alkylene oxides III with MeNHCH2CO2H and lactonization. 2-MeNHC6H4CO2H reacted with propylene oxide to give IV, which gave 2-(HOCPh2)C6H4NMeCH2CHMeOH (V) on treatment with PhLi. V had an antihistamine activity coeff. of 101 compared to 80 for antistin.

IT **85805-12-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and lactonization of)
RN 85805-12-5 HCAPLUS
CN Glycine, N-(2-hydroxy-2,2-diphenylethyl)-N-methyl- (9CI) (CA INDEX NAME)

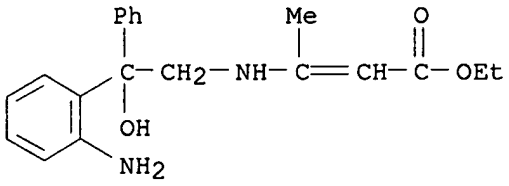


L28 ANSWER 24 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1976:508614 HCAPLUS
DN 85:108614
TI Synthesis of some 1H-1,3-benzodiazepines
AU Taylor, John B.; Tully, W. Roger
CS Roussel Lab. Ltd., Swindon, Engl.
SO J. Chem. Soc., Perkin Trans. 1 (1976), (12), 1331-8
CODEN: JCPRB4
DT Journal
LA English
GI

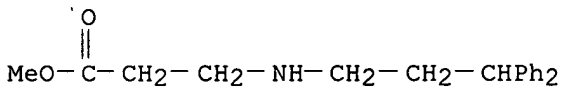


I

AB 3,4-Dihydro-1H-1,3-benzodiazepine-2,5-dione (I) was prepd. from o-nitroacetophenone. The critical step was the reaction of 2,2'-diaminoacetophenone with 1,1'-carbonyldiimidazole to give 77% N-(o-aminophenacylaminocarbonyl)imidazole which cyclized readily in hot H2O to give 88% I. The reactivity at positions 2, 5, and 7 was investigated. Attempts to introduce a 4,5-double bond resulted in rearrangement to quinolines and indoles.
IT **60331-02-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, and cycloaddn. with carbonyldiimidazole)
RN 60331-02-4 HCAPLUS
CN 2-Butenoic acid, 3-[[2-(2-aminophenyl)-2-hydroxy-2-phenylethyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

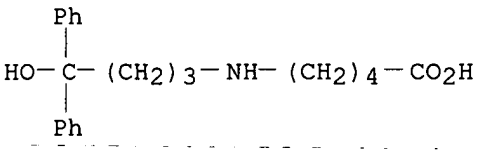


L28 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1973:38037 HCAPLUS
DN 78:38037
TI Potential hypotensive compounds. Substituted 3-aminopropionates and 3-aminopropionohydroxamic acids
AU Biggs, D. F.; Coutts, R. T.; Selley, M. L.; Towill, G. A.
CS Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, Alberta, Can.
SO J. Pharm. Sci. (1972), 61(11), 1739-45
CODEN: JPMSAE
DT Journal
LA English
AB Most of the 48 3-aminoproprionate esters studied were synthesized by addn. of an amine across the .alpha.,.beta.-double bond of Me acrylate [96-33-3], Me methacrylate [80-62-6], or Me crotonate [18707-60-3], while the remainder were obtained by interaction of 1 mole of a 3-bromopropionic ester with 2 moles of the corresponding amine. Twenty-six 3-aminopropionohydroxamic acid hydrochlorides were prepd. by treatment of the appropriate amino ester with hydroxylamine-HCl [5470-11-1] in MeOH. Many of the compds. such as 2-methyl-3-[(2-phenylethyl)amino]propanoic acid Me ester [6297-67-2], 3,3'-[(2-phenylethyl)imino]bispropanoic acid dimethyl ester [38129-46-3], N-[3-(hydroxyamino)-2-methyl-3-oxopropyl]heptanaminium chloride [38129-47-4], and N-[3-(hydroxyamino)-3-oxopropyl]-2-(2-phenylethyl)benzeneethanaminium chloride [38202-84-5] possessed hypotensive properties but of very short duration. 2-Methyl-3-(octylamino)propanoic acid Me ester [29228-46-4] was the most active, and at 4 mg/kg i.v. decreased the blood pressure of rats by an av. of 52% for 12 min. Some of the compds. were screened for their ability to protect mice against a lethal dose of diisopropylfluorophosphate [55-91-4], but none was active.
IT **40871-14-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hypotensive effect of)
RN 40871-14-5 HCAPLUS
CN .beta.-Alanine, N-(3,3-diphenylpropyl)-, methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2002 ACS
AN 1973:23847 HCAPLUS
DN 78:23847
TI Metabolism of diphenidol. Urinary products in humans and dogs
AU Kaiser, Carl; Swagzdis, James E.; Flanagan, Thomas L.; Lester, Bruce M.;

Burghard, Garth L.; Green, Harry; Zirkle, Charles L.
CS Res. Dev. Div., Smith Kline and French Lab., Philadelphia, Pa., USA
SO J. Med. Chem. (1972), 15(11), 1146-50
CODEN: JMCMAR
DT Journal
LA English
AB The principle metabolite of diphenidol (I) [972-02-1] in dogs and humans was N-(4,4-diphenyl-4-hydroxybutyl)-.delta.-aminovaleric acid (II) [**37439-33-1**]. More than 50% of the radioactivity in orally administered I-.alpha.-14C was excreted in the urine as II, along with only 5-10% of unchanged I. Smaller amts. of I gucuronide, a phenolic deriv. of I, a lactam of II, and their glucuronides were also detected in urine of both species. Neither II nor its lactam afforded I-like protection against apomorphine-induced emesis in dogs. The structure of II was confirmed by comparison with synthetic II, prepd. by (1) reaction of 2-piperidone with 2-(3-chloropropyl)-2-phenyl-1,3-dioxolane in DMF in the presence of NaH, (2) hydrolysis of the cyclic ketal with HCl to form 4-(2-ketopiperidinyl)butyrophenone, (3) reaction with PhMgBr, and (4) hydrolysis of the lactam with Ba(OH)2.
IT **37439-33-1**
RL: FORM (Formation, nonpreparative)
(formation of, as diphenidol metabolite)
RN 37439-33-1 HCAPLUS
CN Pentanoic acid, 5-[(4-hydroxy-4,4-diphenylbutyl)amino]- (9CI) (CA INDEX NAME)



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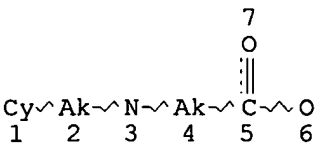


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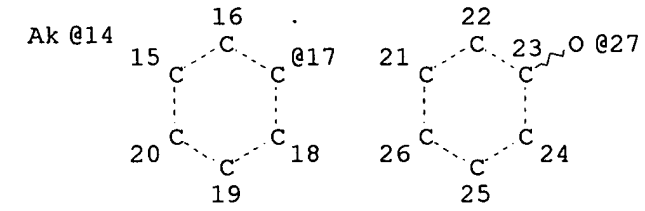

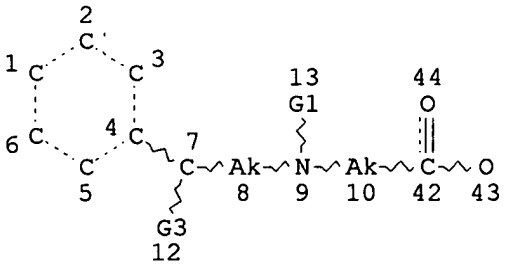


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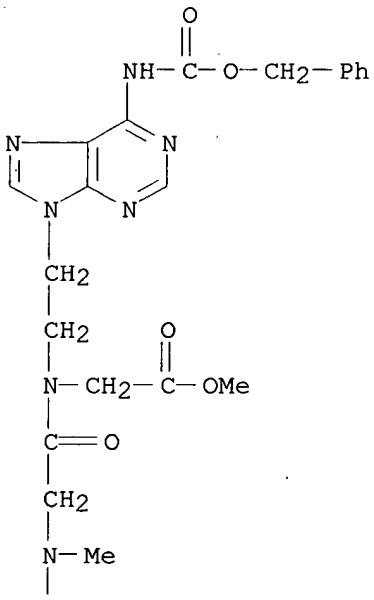
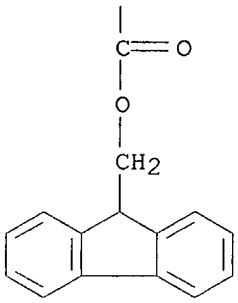
L29 ANSWER 1 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:279228 HCAPLUS
DN 135:46416
TI Synthesis of N-Boc and N-Fmoc dipeptoids with nucleobase residues as peptoid nucleic acid monomers
AU Wu, Yun; Xu, Jie-Cheng; Liu, Jing; Jin, You-Xing
CS Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SO Tetrahedron (2001), 57(16), 3373-3381
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
AB The synthesis of Boc and Fmoc protected peptoid nucleic acid monomers bearing thymine, adenine, or guanine on the side chain is described. These nucleobases were attached to the amino group of glycine via an ethylene linkage using the Mitsunobu reaction, except cytosine, which was attached using alkylation. After deprotection, these amino acids have been used for synthesizing N-Boc and N-Fmoc dipeptoids.
IT **344414-19-3P 344414-20-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of dipeptoid nucleic acid monomers with backbone N-protecting groups)
RN 344414-19-3 HCAPLUS
CN Glycine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-N-methylglycyl-N-[2-[6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

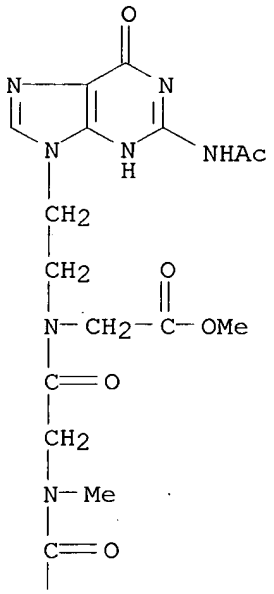


PAGE 2-A



RN 344414-20-6 HCAPLUS
CN Glycine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-N-methylglycyl-N-[2-[2-(acetylamino)-1,6-dihydro-6-oxo-9H-purin-9-yl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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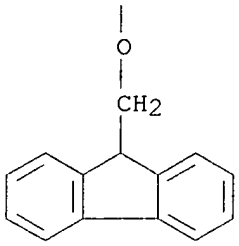
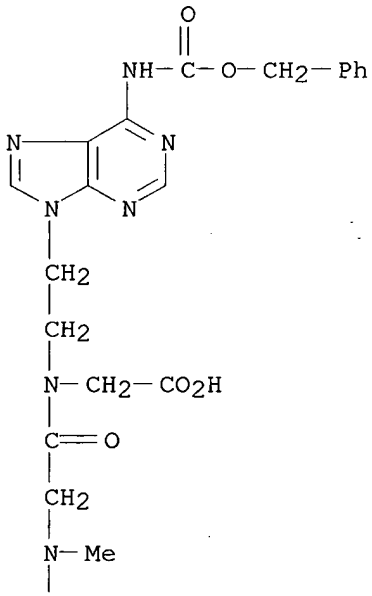


IT **344414-22-8P 344414-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of dipeptoid nucleic acid monomers with backbone N-protecting groups)
RN 344414-22-8 HCAPLUS
CN Glycine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-N-methylglycyl-N-[2-[6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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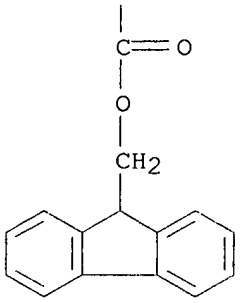
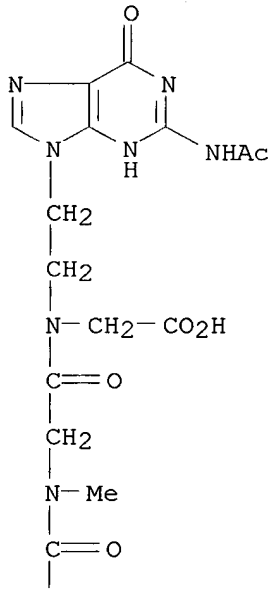
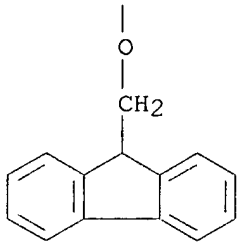


RN 344414-23-9 HCAPLUS
CN Glycine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-N-methylglycyl-N-[2-[2-(acetylamino)-1,6-dihydro-6-oxo-9H-purin-9-yl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





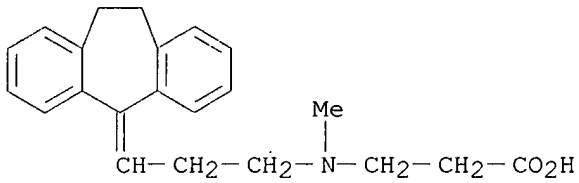
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 2 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:383927 HCAPLUS
DN 133:34425
TI Pharmaceutical compositions containing N-substituted azaheterocyclic compounds for the treatment of indications related to angiogenesis
IN Hansen, Anker Jon; Jorgensen, Tine Krogh; Olsen, Uffe Bang
PA Novo Nordisk A/S, Den.
SO PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

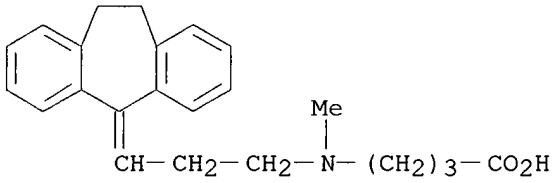
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000032193	A1	20000608	WO 1999-DK671	19991201
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1135129	A1	20010926	EP 1999-957964	19991201
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	DK 1998-1586	A	19981202		
	US 1998-111445	P	19981208		
	WO 1999-DK671	W	19991201		

OS MARPAT 133:34425
AB The present invention relates to the use of N-substituted azaheterocyclic compds. or salts thereof, for the treatment of conditions related to angiogenesis. N-substituted azaheterocyclic compds. decreased the vessel area of neovascularization of mouse cornea by 30-50%. A tablet contained a N-substituted azaheterocyclic compd. 100, silicone dioxide 1.5, microcryst. cellulose 70, modified cellulose gum 7.5, in the core, and hydroxypropyl Me cellulose 9, and Mywacett 9-40T 0.9 mg in the coating.
IT **69436-99-3 183476-92-8 273751-35-2**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. contg. N-substituted azaheterocyclic compds.

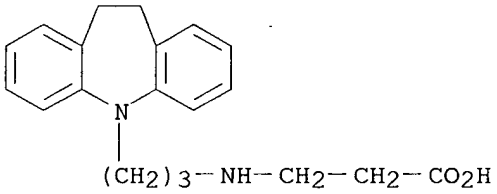
for treatment of indications related to angiogenesis)
RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 183476-92-8 HCAPLUS
CN Butanoic acid, 4-[[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



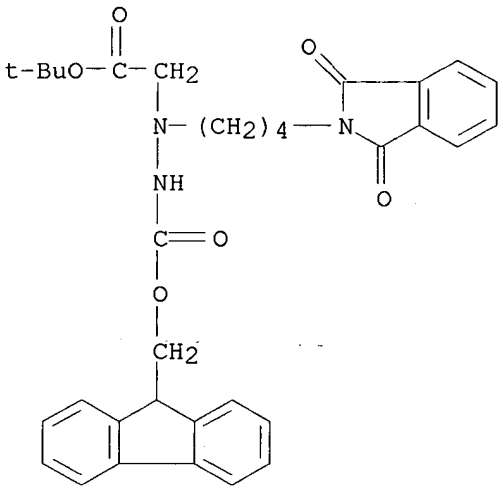
RN 273751-35-2 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]- (9CI) (CA INDEX NAME)



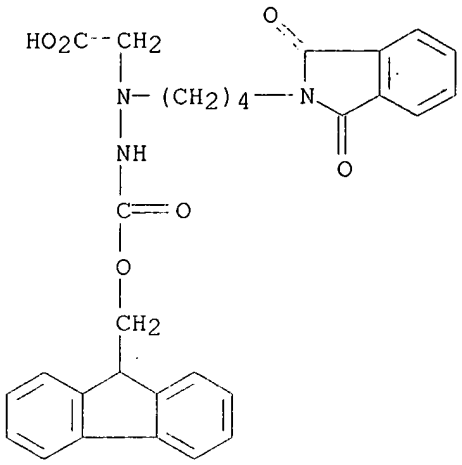
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 3 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:246886 HCAPLUS
DN 133:59045
TI New potential monomers for solid phase synthesis of hydrazinopeptoids: the N.alpha.-substituted-N.beta.-protected hydrazinoglycines and hydrazinoglycinals
AU Cheguillaume, Arnaud; Doubli-Bounoua, Ismahel; Baudy-Floch, Michele; Le Grel, Philippe
CS UMR CRNS 6510, Univ. Rennes I, Rennes, 35042, Fr.
SO Synlett (2000), (3), 331-334
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal

LA English
OS CASREACT 133:59045
AB Various N.alpha.-substituted-N.beta.-protected hydrazinoglycinates (I), easily prepd. from N.alpha.-substituted-N.beta.-protected hydrazine and esters of bromoacetate, are described as precursors of new potential monomers for solid phase synthesis. An easily attainable deprotection route of I affords the N.alpha.-substituted-N.beta.-protected hydrazinoglycines, or the N.alpha.-substituted-hydrazino glycinates. Redn. and oxidn. of I lead to N.alpha.-substituted-N.beta.-protected hydrazino glycinals.
IT **276672-52-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(N.alpha.-substituted-N.beta.-protected hydrazinoglycines and hydrazinoglycinals as monomers for solid phase synthesis of hydrazinopeptoids)
RN 276672-52-7 HCAPLUS
CN Hydrazinecarboxylic acid, 2-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]-2-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)



IT **276672-58-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(N.alpha.-substituted-N.beta.-protected hydrazinoglycines and hydrazinoglycinals as monomers for solid phase synthesis of hydrazinopeptoids)
RN 276672-58-3 HCAPLUS
CN Hydrazinecarboxylic acid, 2-(carboxymethyl)-2-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]-, 1-(9H-fluoren-9-ylmethyl) ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

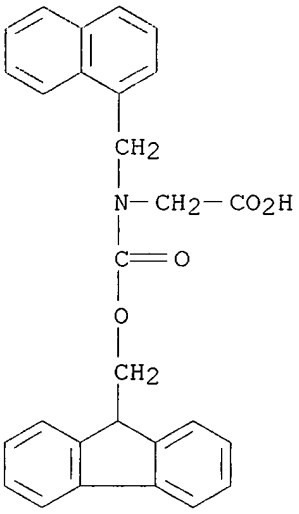
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 4 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:144132 HCAPLUS
DN 132:152142
TI Synthesis of peptides with N-substituted glycines as luteinizing hormone-releasing hormone inhibitory analogs for treatment of hormone-dependent tumors.
IN Dechantsreiter, Michael; Kessler, Horst; Bernd, Michael; Kutscher, Bernhard; Beckers, Thomas
PA Asta Medica A.-G., Germany
SO Ger. Offen., 32 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 19941248	A1	20000302	DE 1999-19941248	19990831
PRAI DE 1998-19839817		19980901		

OS MARPAT 132:152142
AB Title decapeptide compds. in which one or two glycine amine groups have been substituted with side-chain equiv. of natural or non-natural amino acids were prepd. as analogs of LH-RH, for use in treating hormone-dependent tumors or for LH-RH suppression therapies (no data). Thus, amino acid substitutes were prepd. by, for example, alkylation of an amine such as 4-Cl-C6H4-NH2 with BrCH2COOEt, or amination of CHOCO2H with RNH(CH2)2OC(CH3)3 (R = protecting group). The amino acid substitutes could then be used in solid-phase synthesis (BOC or Fmoc chem.) to prep. fragments for soln. coupling to give the final decapeptides.
IT **258333-01-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of N-substituted glycines for use in prepn. of peptides as LH-releasing hormone inhibitory analogs for treatment of

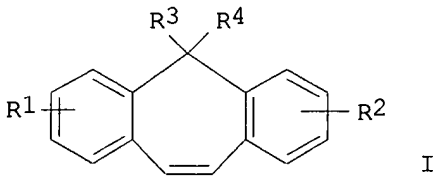
hormone-dependent tumors)
RN 258333-01-6 HCAPLUS
CN Glycine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-N-(1-naphthalenylmethyl)-(9CI) (CA INDEX NAME)



L29 ANSWER 5 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1999:312695 HCAPLUS
DN 131:27963
TI Dibenzocycloheptenes and aldose reductase inhibitors for prevention and treatment of diabetic complications
IN Inoue, Atsushi; Choi, Ying-She
PA Senju Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11130713	A2	19990518	JP 1997-309706	19971023

OS MARPAT 131:27963
GI



I

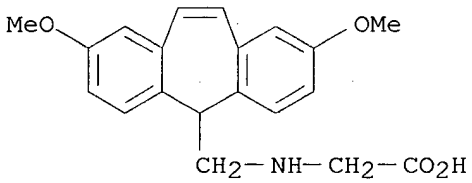
AB Title inhibitors contain dibenzocycloheptenes I [R1, R2 = OH, (aryl-substituted) lower alkoxy, halo; if R1 or R2 = halo, then the other

= OH; if R3 or R4 = H, the other = CH2OH, lower alkylaminomethyl, carboxy(lower alkyl)aminomethyl, dioxothiazolidylidenemethyl, CO2H, CHO, oxo-4H-oxadiazolyl; R3R4 = O, ring] or their salts. 2-[.beta.-(3-Methoxyphenyl)ethyl]-4-methoxybenzoic acid was cyclized, dehydrogenated, and demethylated to give I (R1 = 2-OH, R2 = 8-OMe, R3R4 = O), which in vitro inhibited rat lens aldose reductase with IC50 of 25 .mu.M.

IT **226897-15-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of dibenzocycloheptenes as aldose reductase inhibitors for prevention and treatment of diabetic complications)

RN 226897-15-0 HCAPLUS

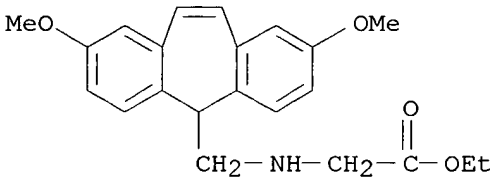
CN Glycine, N-[(2,8-dimethoxy-5H-dibenzo[a,d]cyclohepten-5-yl)methyl]- (9CI) (CA INDEX NAME)



IT **226897-24-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of dibenzocycloheptenes as aldose reductase inhibitors for prevention and treatment of diabetic complications)

RN 226897-24-1 HCAPLUS

CN Glycine, N-[(2,8-dimethoxy-5H-dibenzo[a,d]cyclohepten-5-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 6 OF 34 HCAPLUS COPYRIGHT 2002 ACS

AN 1998:789498 HCAPLUS

DN 130:164074

TI Monoclonal Antibody-Based ELISAs for Part-per-Billion Determination of Polycyclic Aromatic Hydrocarbons: Effects of Haptens and Formats on Sensitivity and Specificity

AU Li, Kai; Chen, Rongliang; Zhao, Bitao; Liu, Mei; Karu, Alexander E.; Roberts, Victoria A.; Li, Qing X.

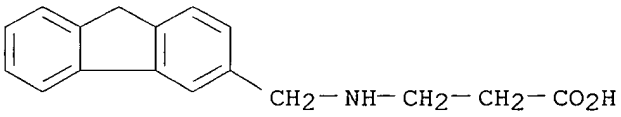
CS Department of Environmental Biochemistry, University of Hawaii at Manoa, Honolulu, HI, 96822, USA

SO Anal. Chem. (1999), 71(2), 302-309
CODEN: ANCHAM; ISSN: 0003-2700

PB American Chemical Society

DT Journal

LA English
AB As a first step toward developing sensitive enzyme-linked immunosorbent assays (ELISAs) for multianalyte detection of polycyclic arom. hydrocarbons (PAHs), haptens with different lengths of carboxylic acid spacers at various positions were derived from naphthalene, fluorene, anthracene, phenanthrene, pyrene, fluoranthene, chrysene, and benzo[a]pyrene (BaP). These haptens were coupled with bovine serum albumin (BSA) to form competitor conjugates. All of these haptens were recognized to different extents by monoclonal antibodies (MAbs) 4D5 and 10C10 originally derived by Gomes and Santella (Chem. Res. Toxicol. 1990, 3, 307-310). The most sensitive indirect ELISAs were obtained by coating wells with the least competitive conjugates. Direct ELISAs using horseradish peroxidase conjugates of pyrene and BaP were less sensitive. The MAbs bound BaP with spacers at either C1 or C6. The cross-reactivity profiles of the eight PAHs were different with each PAH-BSA conjugate used as coating antigen. The ELISA results for BaP closely correlated with those by gas chromatog. (GC), but the detection limit of the ELISA was .apprx.150-fold more sensitive than that of GC, with 2-600 nM spike recoveries of 80-127% from human urine and canal and tap water.
IT **220339-13-9**
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(monoclonal antibody-based ELISAs for part-per-billion detn. of polycyclic arom. hydrocarbons in relation to effects of haptens and formats on sensitivity and specificity)
RN 220339-13-9 HCAPLUS
CN .beta.-Alanine, N-(9H-fluoren-3-ylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

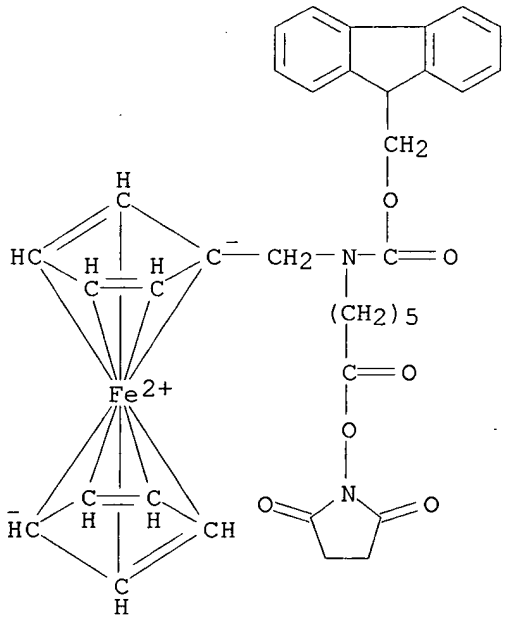
L29 ANSWER 7 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1998:283803 HCAPLUS
DN 129:73271
TI Facile derivatization of glassy carbon surfaces by N-hydroxysuccinimide esters in view of attaching biomolecules
AU Anne, Agnes; Blanc, Bernard; Moiroux, Jacques; Saveant, Jean Michel
CS Laboratoire d'Electrochimie Moleculaire, Unite Mixte de Recherche Universite, CNRS No. 7591, Universite Denis Diderot, Paris, 75251, Fr.
SO Langmuir (1998), 14(9), 2368-2371
CODEN: LANGD5; ISSN: 0743-7463
PB American Chemical Society
DT Journal
LA English
AB The reaction of N-hydroxysuccinimide (NHS) esters with freshly polished glassy carbon surfaces offers a facile and versatile method of derivatization. Surface concns. larger than 10-10 mol/cm2 can thus be easily achieved. They can be further increased when polishing is carried out in the presence of ammonia, which also improves their reproducibility. The derivatization results from the formation of a covalent peptide linkage by reaction of the NHS ester with superficial amino groups on the

glassy carbon surface. The peptide linkage is remarkably stable in time and can only be hydrolyzed in very strong basic media. 9-Fluorenylmethoxycarbonyl chloride protection, followed by prepn. of the NHS ester, by surface derivatization and by mild deprotection allows the grafting of a mol. that contains an amino group located remotely from the electrode surface, thus opening a route to the attachment of a large variety of biomols., for which NHS esters are available, in a position where their degrdn. should be avoided or minimized.

IT **209053-56-5**, N-Succinimidyl [N-(ferrocenylmethyl)-N-(9-fluorenylmethoxycarbonyl)-6-amino]hexanoate
RL: RCT (Reactant)
(with amino groups on glassy carbon in facile derivatization of glassy carbon surfaces for electrodes)

RN 209053-56-5 HCAPLUS

CN Ferrocene, [[[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl][(9H-fluoren-9-ylmethoxy)carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



L29 ANSWER 8 OF 34 HCAPLUS COPYRIGHT 2002 ACS

AN 1997:623152 HCAPLUS

DN 127:262691

TI Preparation of nitrogenous tricyclic compounds as allergy inhibitors

IN Miyamoto, Mitsuaki; Yoshiuchi, Tatsuya; Sato, Keizo; Kaino, Makoto; Tanaka, Masayuki; Soejima, Motohiro; Moriya, Katsuhiro; Sakuma, Yoshinori; Yamada, Koji; Harada, Kokichi; Nishizawa, Yukio; Kobayashi, Seiichi; Okita, Makoto; Katayama, Koichi

PA Eisai Co., Ltd., Japan; Miyamoto, Mitsuaki; Yoshiuchi, Tatsuya; Sato, Keizo; Kaino, Makoto; Tanaka, Masayuki; Soejima, Motohiro; Moriya, Katsuhiro; Sakuma, Yoshinori; et al.

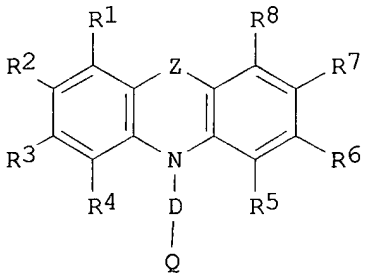
SO PCT Int. Appl., 175 pp.
CODEN: PIXXD2

DT Patent

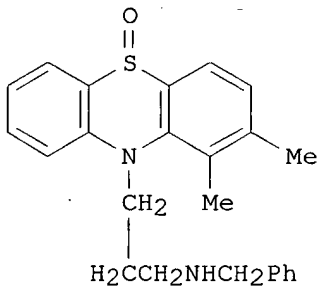
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9733871	A1	19970918	WO 1997-JP789	19970313
	W: AU, CA, CN, HU, JP, KR, MX, NO, NZ, RU, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2248820	AA	19970918	CA 1997-2248820	19970313
	AU 9719399	A1	19971001	AU 1997-19399	19970313
	EP 889037	A1	19990107	EP 1997-907297	19970313
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	CN 1216982	A	19990519	CN 1997-194202	19970313
	NO 9804217	A	19981112	NO 1998-4217	19980911
	US 6333322	B1	20011225	US 1998-125451	19980921
PRAI	JP 1996-55628	A	19960313		
	WO 1997-JP789	W	19970313		

OS MARPAT 127:262691
GI



I



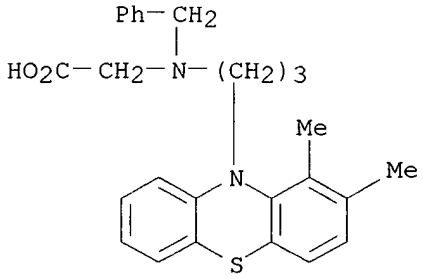
II

AB The title compds. I [D = alkylene; R1 - R8 = hydrogen, hydroxy, cyano, nitro, optionally substituted carbamoyl, halogeno, lower alkyl optionally substituted by halogeno, etc.; Z = S, SO, etc. ; and Q represents, for example, NR20R21 (where R20, R21 = hydrogen, lower alkyl optionally substituted by halogeno, optionally substituted aryl, optionally substituted arylalkyl, optionally substituted heteroaryl, or optionally substituted heteroarylalkyl, or NR20R21 = three- to eight-membered ring)] are prepd. I are effective in the prevention and treatment of diseases in which chem. transmitters such as histamine and leukotriene participate, for example, asthma, allergic rhinitis, atopic dermatitis, hives, hay fever, gastrointestinal allergy, and dietary allergy. In an in vitro test

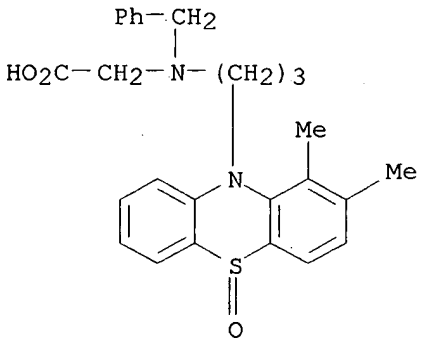
for inhibition of antigen-induced histamine release from basophils, the title compd. II showed IC50 of 10 - 30 .mu.M.

IT **196094-39-0P 196095-65-5P 196095-91-7P 196095-93-9P 196095-94-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogenous tricyclic compds. as allergy inhibitors)

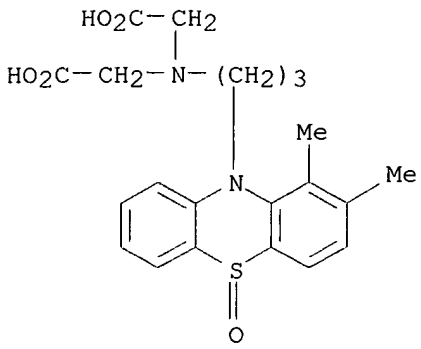
RN 196094-39-0 HCAPLUS
CN Glycine, N-[3-(1,2-dimethyl-10H-phenothiazin-10-yl)propyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



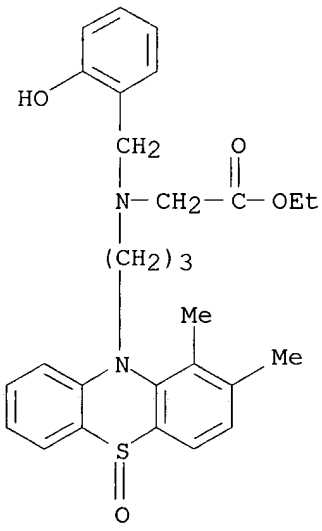
RN 196095-65-5 HCAPLUS
CN Glycine, N-[3-(1,2-dimethyl-5-oxido-10H-phenothiazin-10-yl)propyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



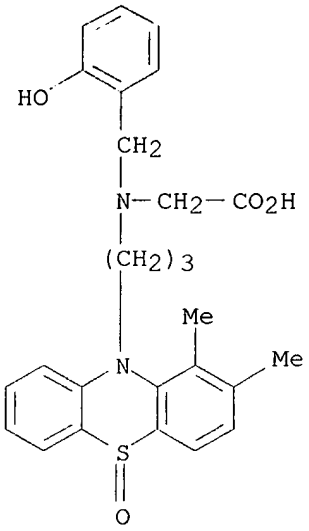
RN 196095-91-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-[3-(1,2-dimethyl-5-oxido-10H-phenothiazin-10-yl)propyl]- (9CI) (CA INDEX NAME)



RN 196095-93-9 HCAPLUS
CN Glycine, N-[3-(1,2-dimethyl-5-oxido-10H-phenothiazin-10-yl)propyl]-N-[(2-hydroxyphenyl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 196095-94-0 HCAPLUS
CN Glycine, N-[3-(1,2-dimethyl-5-oxido-10H-phenothiazin-10-yl)propyl]-N-[(2-hydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

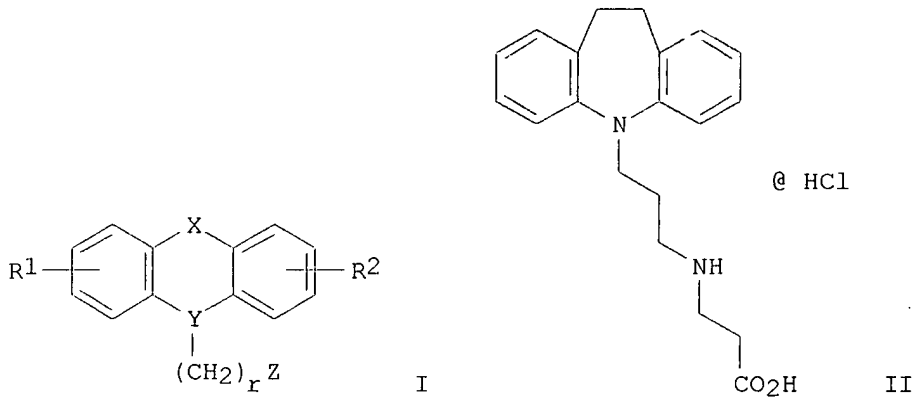


L29 ANSWER 9 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1996:708300 HCAPLUS
DN 125:328528
TI Preparation of heterocyclic tricyclic analgesics, antidiabetics and antiinflammatory agents
IN Madsen, Peter; Andersen, Knud Erik; Doerwald, Florenzio Zaragossa; Joergensen, Tine Krogh; Andersen, Henrik Sune; Hohlweg, Rolf; Olsen, Uffe Bang
PA Novo Nordisk A/s, Den.
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9631481	A1	19961010	WO 1996-DK141	19960401
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML				
	US 5962449	A	19991005	US 1996-623447	19960328
	CA 2217198	AA	19961010	CA 1996-2217198	19960401
	AU 9652706	A1	19961023	AU 1996-52706	19960401
	EP 820443	A1	19980128	EP 1996-909078	19960401
	EP 820443	B1	20010919		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 11503129	T2	19990323	JP 1996-529870	19960401
	AT 205833	E	20011015	AT 1996-909078	19960401
	ZA 9602733	A	19961024	ZA 1996-2733	19960404
PRAI	DK 1995-407	A	19950407		
	DK 1995-1002	A	19950911		
	WO 1996-DK141	W	19960401		

OS MARPAT 125:328528

GI



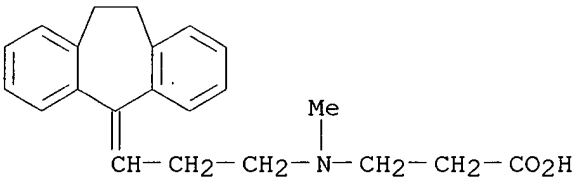
I II

AB The title compds. [I; R1, R2 = H, halogen, CF3, OH, alkyl, alkoxy; X = O, S, CH2CH2, (un)substituted NH, CH2O, OCH2, S(:O), etc.; Y = NCH2, CHCH2, C:CH; Z = (un)substituted 2-pyridylamino, (un)substituted cyclohexylamino, etc.; r = 1-3], useful for the clin. treatment of painful, hyperalgesic and/or inflammatory conditions in which C-fibers play a pathophysiol. role by eliciting neurogenic pain or inflammation, and for the treatment of noninsulin-dependent diabetes mellitus (no data), are prepd. and a I-contg. formulation presented. Thus, dihydrodibenz[b,f]azepine II (m.p. 114-117.degree.) was prepd. in 4 steps from 10,11-dihydro-5H-dibenz[b,f]azepine and demonstrated a 36% inhibition of pain in a mouse formalin-induced pain model at 0.1 mg/kg.

IT **69436-99-3P 183476-85-9P 183476-92-8P 183476-93-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic tricyclic analgesics, antidiabetics and antiinflammatory agents)

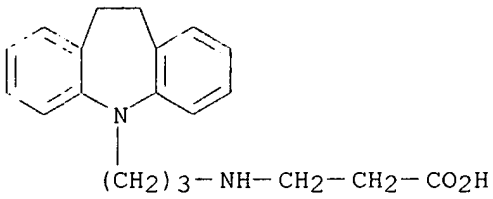
RN 69436-99-3 HCAPLUS

CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



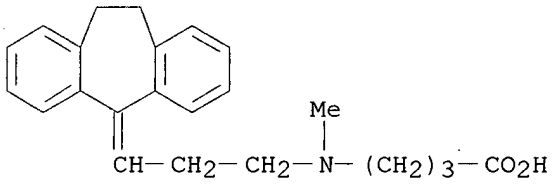
RN 183476-85-9 HCAPLUS

CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

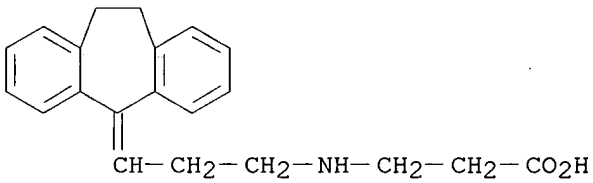


● HCl

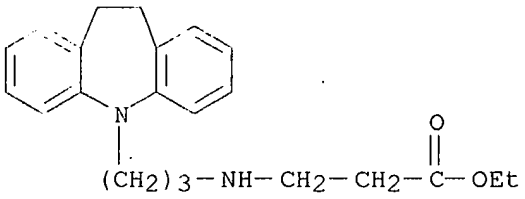
RN 183476-92-8 HCAPLUS
CN Butanoic acid, 4-[[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



RN 183476-93-9 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]- (9CI) (CA INDEX NAME)



IT **183476-99-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of heterocyclic tricyclic analgesics, antidiabetics and antiinflammatory agents)
RN 183476-99-5 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



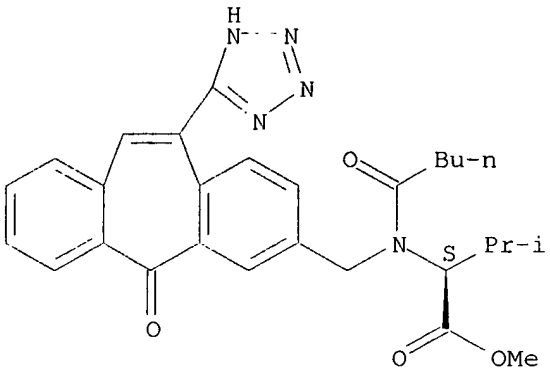
● HCl

L29 ANSWER 10 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:881451 HCAPLUS
DN 123:286044
TI Preparation of tetrazolyldibenzocycloheptene derivatives as angiotensin II antagonists
IN Fujishita, Toshio; Kyama, Ryuichi; Fujimoto, Masabumi; Hara, Mariko; Pponma, Tsunetoshi
PA Shionogi Seiyaku Kk, Japan
SO Jpn. Kokai Tokkyo Koho, 40 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 07165689	A2	19950627	JP 1994-257207	19941021
PRAI JP 1993-263933		19931021		

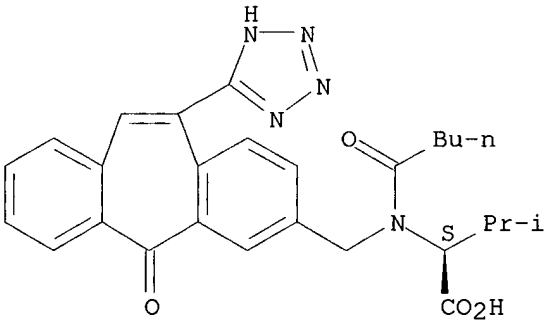
OS MARPAT 123:286044
GI For diagram(s), see printed CA Issue.
AB The title compds. I [X = CO, etc.; Y = tetrazolyl, etc.; ring A = (un)substituted benzene ring, etc.; Z = (un)substituted imidazolyl, etc.] are prepd. In an in vitro test for angiotensin II antagonism, the title compds. II and III (prepn. given) showed Ki values of 1 and 15 nM, resp. The Ki values of 18 compds. of this invention in the above test are given in a table in this document.
IT **169270-85-3P 169270-90-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tetrazolyldibenzocycloheptene derivs. as angiotensin II antagonists)
RN 169270-85-3 HCAPLUS
CN L-Valine, N-(1-oxopentyl)-N-[[5-oxo-11-(1H-tetrazol-5-yl)-5H-dibenzo[a,d]cyclohepten-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



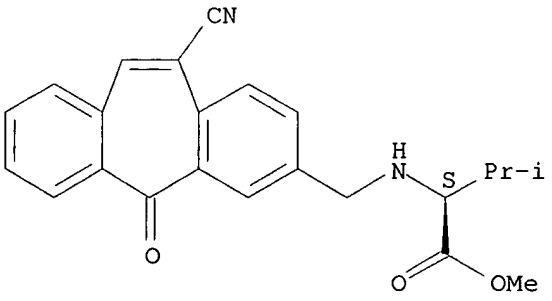
RN 169270-90-0 HCAPLUS
CN L-Valine, N-(1-oxopentyl)-N-[[5-oxo-11-(1H-tetrazol-5-yl)-5H-dibenzo[a,d]cycloheptен-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **169270-83-1P 169270-84-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of tetrazolyldibenzocycloheptene derivs. as angiotensin II antagonists)
RN 169270-83-1 HCAPLUS
CN L-Valine, N-[(11-cyano-5-oxo-5H-dibenzo[a,d]cycloheptен-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

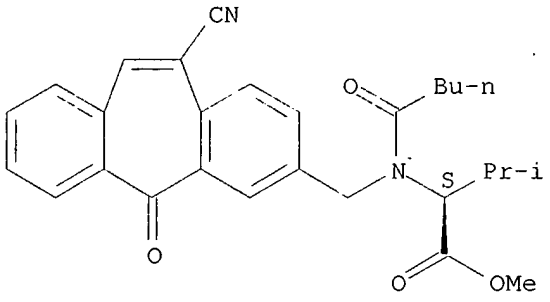
Absolute stereochemistry.



RN 169270-84-2 HCAPLUS

CN L-Valine, N-[(11-cyano-5-oxo-5H-dibenzo[a,d]cyclohepten-3-yl)methyl]-N-(1-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)

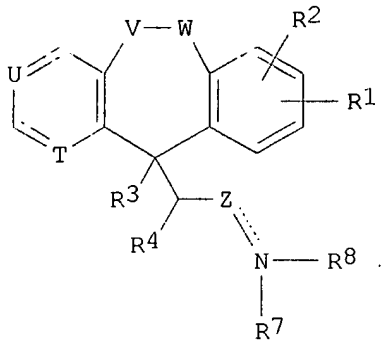
Absolute stereochemistry.



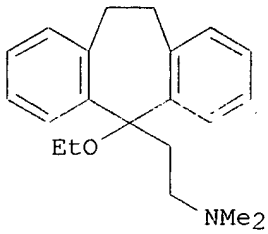
L29 ANSWER 11 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:835588 HCAPLUS
DN 123:227838
TI Tricyclic derivatives, useful as inhibitors of TNF-.alpha., and pharmaceutical compositions containing them.
IN Ting, Pauline C.; Solomon, Daniel L.; Friary, Richard J.; Villani, Frank J.; Piwinski, John J.; Lee, Joe F.; Seidl, Vera A.; Jakway, James P.; Vashi, Dhiru B.
PA Schering Corp., USA
SO PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9515939	A1	19950615	WO 1994-US13662	19941205
	W: JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5538986	A	19960723	US 1993-162744	19931206
	EP 733035	A1	19960925	EP 1995-903619	19941205
	EP 733035	B1	19990331		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 09500656	T2	19970121	JP 1994-516223	19941205
	JP 2793915	B2	19980903		
	AT 178313	E	19990415	AT 1995-903619	19941205
	ES 2131300	T3	19990716	ES 1995-903619	19941205
	US 5767120	A	19980616	US 1995-479418	19950606
	CA 2175287	AA	19971030	CA 1996-2175287	19960429
PRAI	US 1993-162744		19931206		
	WO 1994-US13662		19941205		

OS MARPAT 123:227838
GI



I

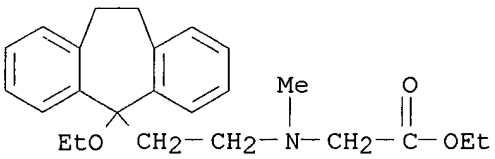


II

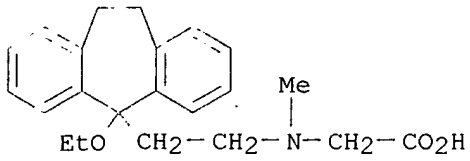
AB The invention discloses tricyclic compds. I and their pharmaceutically acceptable salts or solvates [in which 1 of T and U = CH, other = N or CH; 1 of V and W = CH2, other = O or CH2; R1, R2 = H, halo; R3 = alkyl, alkenyl, alkynyl, aryl, alkaryl, aralkyl, cycloalkyl, acyloxymethyl, alkoxy, alkoxymethyl, or alkyl substituted with cycloalkyl; R4 = H, alkyl, alkenyl, alkoxy, or OH; Z = CH, CH2C(R5), bond, CH2, CH:CH, CH2CR5R6; R5, R6 = H, alkyl; R7, R8 = H, alkyl, alkenyl, alkynyl, aryl, OH, alkoxy, alkanoyl, alkoxycarbonyl, etc.; or R7R8 together = OR9 or certain 5- or 6-membered rings; R9 = H, alkyl]. Also disclosed are pharmaceutical compns. contg. I, methods for inhibiting tumor necrosis factor-.alpha. (TNF-.alpha.) using I, and methods for treating septic shock, inflammation, or allergic disease using I. For example, reaction of 5-ethoxydibenzosuberone with KNH2 in liq. NH3 at -33.degree., followed by reaction of the resultant salt with ClCH2CH2NMe2, gave title compd. II in 48% yield. In a test for inhibition of LPS/galactosamine-induced lethality in mice [septic shock model], II gave complete protection at 25 mg/kg (oral or i.p.). Approx. 100 compds. I (bases and salts) were prepd., claimed, and/or tested. Addnl. test results for inhibition of TNF-.alpha. prodn. by I, both in vitro and in vivo, are described.

IT **168547-83-9P 168547-85-1P 168547-95-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tricyclic derivs. as inhibitors of TNF-.alpha.)

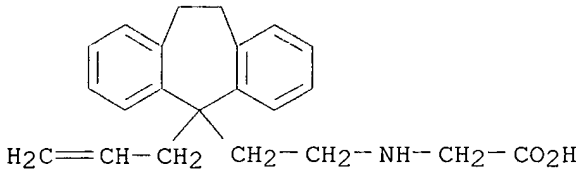
RN 168547-83-9 HCAPLUS
CN Glycine, N-[2-(5-ethoxy-10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 168547-85-1 HCAPLUS
CN Glycine, N-[2-(5-ethoxy-10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)

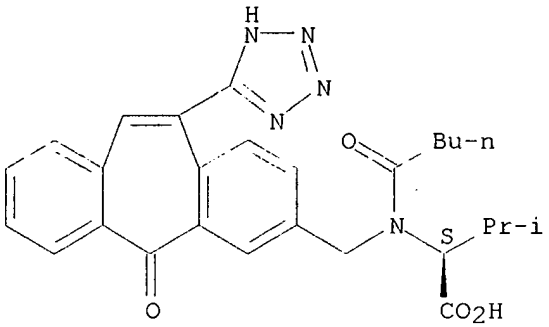


RN 168547-95-3 HCAPLUS
CN Glycine, N-[2-[10,11-dihydro-5-(2-propenyl)-5H-dibenzo[a,d]cyclohepten-5-yl]ethyl]- (9CI) (CA INDEX NAME)



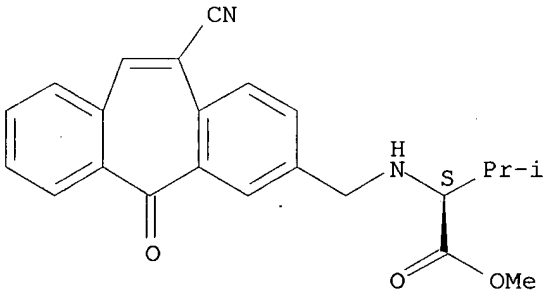
L29 ANSWER 12 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:667003 HCAPLUS
DN 123:284890
TI Novel Angiotensin II Receptor Antagonists. Design, Synthesis, and in Vitro Evaluation of Dibenzo[a,d]cycloheptene and Dibenzo[b,f]oxepin Derivatives. Searching for Bioisosteres of Biphenyltetrazole Using a Three-Dimensional Search Technique
AU Kiyama, Ryuichi; Honma, Tsunetoshi; Hayashi, Kunio; Ogawa, Masayoshi; Hara, Mariko; Fujimoto, Masafumi; Fujishita, Toshio
CS Shionogi Research Laboratories, Shionogi Co. Ltd, Osaka, 553, Japan
SO J. Med. Chem. (1995), 38(14), 2728-41
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Three-dimensional substructure searching (3D search), using the program MACCS-3D, was utilized for designing novel angiotensin II receptor antagonists which contain a bioisostere of the biphenyltetrazole moiety of DuP 753. A 3D query was prepd. from an overlay model of substructures of several potent AII antagonists. The search system retrieved 139 compds. from the database MDDR-3D, which consisted of 29,400 medicinal patent compds. A tricyclic compd. was selected from the retrieved compds. and then evolved by considering steric fitness to the overlay model and synthetic feasibility. Finally, various novel AII antagonists having dibenzo[a,d]cycloheptene or dibenzo[b,f]oxepin were designed and synthesized. The receptor binding activity (Ki) for several members of this series was in the 10-10 M range, demonstrating the ability of 3D search technique to explore new lead structures.
IT **169270-90-0P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of dibenzocycloheptene and dibenzoxepin derivs. as angiotensin II receptor antagonists)
RN 169270-90-0 HCAPLUS
CN L-Valine, N-(1-oxopentyl)-N-[[5-oxo-11-(1H-tetrazol-5-yl)-5H-dibenzo[a,d]cyclohepten-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



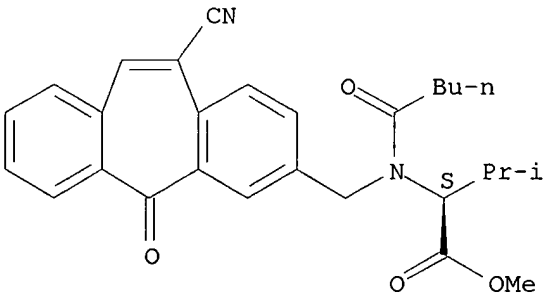
IT **169270-83-1P 169270-84-2P 169270-85-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of dibenzocycloheptene and dibenzoxepin derivs. as angiotensin II receptor antagonists)
RN 169270-83-1 HCAPLUS
CN L-Valine, N-[(11-cyano-5-oxo-5H-dibenzo[a,d]cyclohepten-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 169270-84-2 HCAPLUS
CN L-Valine, N-[(11-cyano-5-oxo-5H-dibenzo[a,d]cyclohepten-3-yl)methyl]-N-(1-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)

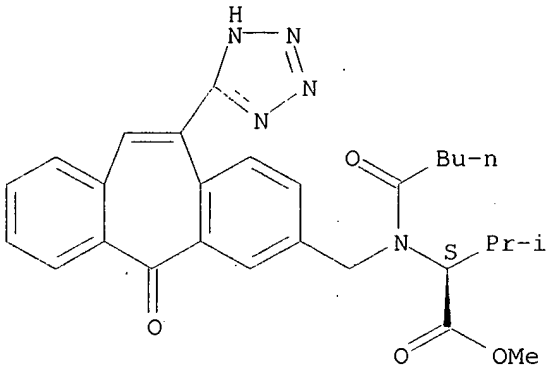
Absolute stereochemistry.



RN 169270-85-3 HCAPLUS

CN L-Valine, N-(1-oxopentyl)-N-[[5-oxo-11-(1H-tetrazol-5-yl)-5H-dibenzo[a,d]cycloheptен-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

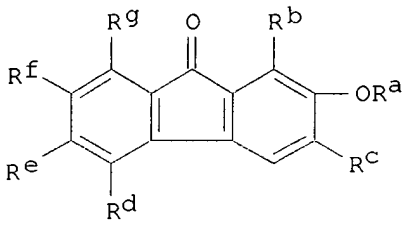
Absolute stereochemistry.



L29 ANSWER 13 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:480301 HCAPLUS
DN 122:239345
TI Preparation of fluorenone derivatives as central or peripheral nerve degeneration repair and protective agents
IN Tanaka, Tatsuyoshi; Sakurai, Yohji; Fujisawa, Nobutaka; Hongoh, Osamu; Nishi, Takao
PA Otsuka Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 159 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9500468	A1	19950105	WO 1994-JP966	19940615
	W: AU, CA, CN, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2142735	AA	19950105	CA 1994-2142735	19940615
	AU 9469819	A1	19950117	AU 1994-69819	19940615
	AU 670696	B2	19960725		
	EP 655992	A1	19950607	EP 1994-918525	19940615
	EP 655992	B1	19981104		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CN 1110875	A	19951025	CN 1994-190385	19940615
	EP 791570	A1	19970827	EP 1997-107083	19940615
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	AT 172956	E	19981115	AT 1994-918525	19940615
	ES 2123139	T3	19990101	ES 1994-918525	19940615
	JP 07061949	A2	19950307	JP 1994-134125	19940616
	JP 2807860	B2	19981008		
	JP 10114697	A2	19980506	JP 1997-283726	19940616
	US 5942641	A	19990824	US 1995-381865	19950207
PRAI	JP 1993-147740		19930618		
	EP 1994-918525		19940615		
	WO 1994-JP966		19940615		

JP 1994-134125 19940616
OS MARPAT 122:239345
GI



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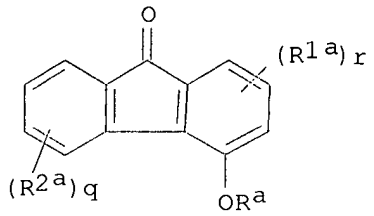
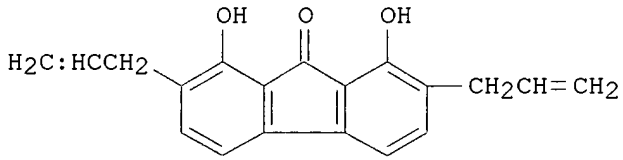


II

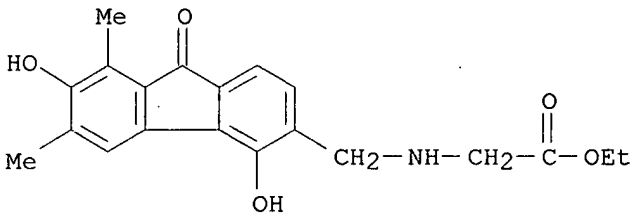


III

AB The title compds. [I; Ra = H, lower alkenyl, Ac; Rb, Rc = H, lower alkenyl, alkyl, halogen, alkylthio, alkenyloxy, (un)substituted aminoalkyl, etc.; Rd-Rg = H, alkenyl, alkyl, halogen, alkoxy, etc.] (II; R1a = Rb, Rc; R2a = Rd-Rg; q = 1-4; r = 1-3), useful as central or peripheral nerve degeneration repair and protective agents, are prepd. and I- and II-contg. formulations presented. Thus, III (m.p. 165.0-167.0.degree.) was prepd. and demonstrated extremely strong neurite sproutings in cerebral cortex-derived nerve cells at 1 x 10-7 M when compared to a control.

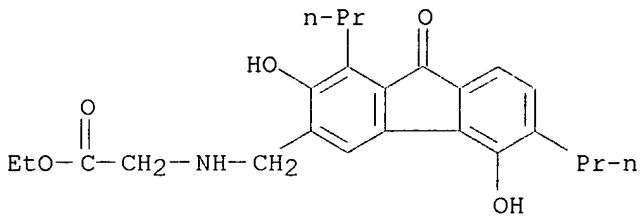
IT **162138-38-7P 162138-41-2P 162138-48-9P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of fluorenone derivs. as central or peripheral nerve degeneration repair and protective agents)

RN 162138-38-7 HCAPLUS
CN Glycine, N-[(4,7-dihydroxy-6,8-dimethyl-9-oxo-9H-fluoren-3-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

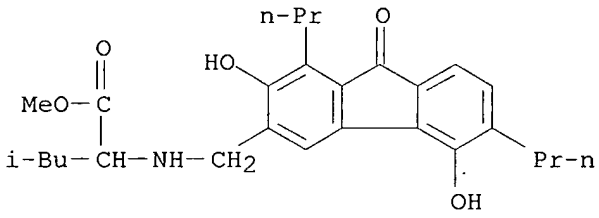


RN 162138-41-2 HCAPLUS

CN Glycine, N-[(2,5-dihydroxy-9-oxo-1,6-dipropyl-9H-fluoren-3-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 162138-48-9 HCAPLUS
CN Leucine, N-[(2,5-dihydroxy-9-oxo-1,6-dipropyl-9H-fluoren-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 14 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:331663 HCAPLUS
DN 123:256741
TI Tricyclic compounds as antagonists of angiotensin II receptors
IN Ohshima, Etsuo; Kanai, Fumihiko; Sato, Hideyuki; Obase, Hiroyuki; Kumazawa, Toshiaki; Takahara, Shiho; Ohno, Tetsuji; Ishikawa, Tomoko; Yamada, Koji
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO U.S., 44 pp. Cont.-in-part of U.S. Ser. No. 996,694, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5378701	A	19950103	US 1993-65916	19930525
	US 5478840	A	19951226	US 1994-294978	19940824
	US 5607955	A	19970304	US 1995-431425	19950501
PRAI	JP 1991-347294	A	19911227		
	US 1992-996694	B2	19921224		
	US 1993-65916	A3	19930525		
	US 1994-294978	A3	19940824		

OS MARPAT 123:256741
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

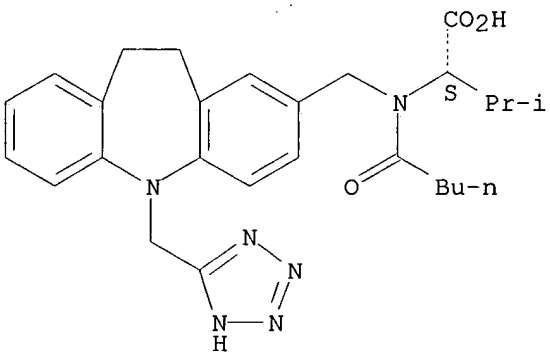
AB A tricyclic compd. is provided, represented by the following formula I wherein R1 represents hydrogen, halogen or lower alkyl; A represents cyano, carboxyl, tetrazolyl, cyano-substituted Ph, carboxyl-substituted Ph or tetrazolyl-substituted phenyl; V represents (CH2)m wherein m is an integer of 0 to 2; W represents II and Q1-Q2-Q3-Q4 represents N:CHCH:CH, CH:CHCH:CH or CH2-CH2-CH2-CH2, III-V and Q represents N or CH; X1-X2-X3 represents CH:CHCH:CH, SCH:CH or CH:CHS; Y represents CH2CH2; and Z1-Z2 represents N(CH2)n wherein n is an integer of 1 to 3 or a pharmaceutically acceptable salt thereof. Thus, e.g., detritylation of the trityltetrazolyl deriv. (prepn. given) with aq. HCl afforded (imidazopyridinylmethyl)(tetrazolylmethyl)dihydrodibenzazepine VI (64% yield). The inhibitory activity (inhibition rate, %) of VI (0.1 .mu.M) against the receptor binding of [125I]AII was 86%. Inhibition test against hypertensive response to AII: 45% for VI. Pharmaceutical formulations were given.

IT **150802-67-8P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tricyclic compds. as antagonists of angiotensin II receptors)

RN 150802-67-8 HCAPLUS

CN L-Valine, N-[[10,11-dihydro-5-(1H-tetrazol-5-ylmethyl)-5H-dibenz[b,f]azepin-2-yl]methyl]-N-(1-oxopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

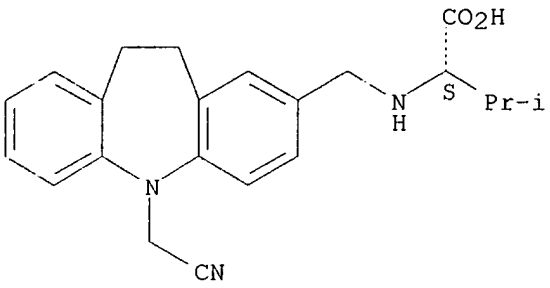


IT **150802-69-0P 150802-70-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(tricyclic compds. as antagonists of angiotensin II receptors)

RN 150802-69-0 HCAPLUS

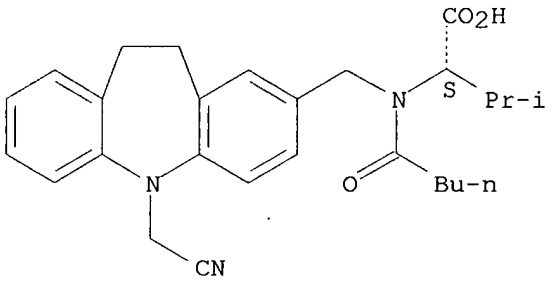
CN L-Valine, N-[[5-(cyanomethyl)-10,11-dihydro-5H-dibenz[b,f]azepin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 150802-70-3 HCAPLUS
CN L-Valine, N-[[5-(cyanomethyl)-10,11-dihydro-5H-dibenz[b,f]azepin-2-yl]methyl]-N-(1-oxopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

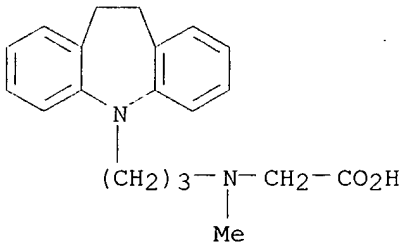


L29 ANSWER 15 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1994:650195 HCAPLUS
DN 121:250195
TI Characterization of Protein-Hapten Conjugates. 1. Matrix-Assisted Laser Desorption Ionization Mass Spectrometry of Immuno BSA-Hapten Conjugates and Comparison with Other Characterization Methods
AU Adamczyk, Maciej; Buko, Alex; Chen, Yon-Yih; Fishpaugh, Jeffrey R.; Gebler, John C.; Johnson, Donald D.
CS Division Organic Chemistry Research (D-9NM), Abbott Laboratories, Abbott Park, IL, 60064, USA
SO Bioconjugate Chem. (1994), 5(6), 631-5
CODEN: BCCHES; ISSN: 1043-1802
DT Journal
LA English
AB Several different low mol. wt. haptens were conjugated to BSA to produce immunogens useful for antibody development. The extent of BSA modification due to covalent attachment of hapten was estd. by matrix-assisted laser desorption ionization mass spectrometry. The av. no. of hapten incorporated into immunogen was detd. from the difference in the measured mol. wts. of the conjugate from nonmodified BSA. The results from mass spectrometry were compared with results obtained from other more traditional methods of immunogen characterization (UV anal., trinitrobenzenesulfonic acid titrns., and gel electrophoresis). In each case the authors were able to calc. the av. no. of hapten covalently bound to BSA for each synthetically prepd. immunogen using matrix-assisted laser desorption ionization mass spectrometry. The other methods presented

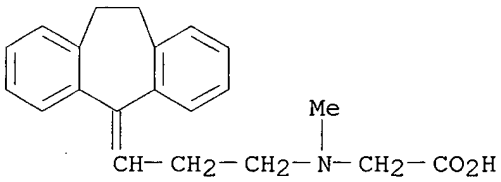
limitations in certain cases.

IT **158446-88-9DP**, albumin conjugates **158446-92-5DP**, albumin conjugates
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(BSA-hapten conjugates characterization by matrix-assisted laser-desorption/ionization mass spectrometry)

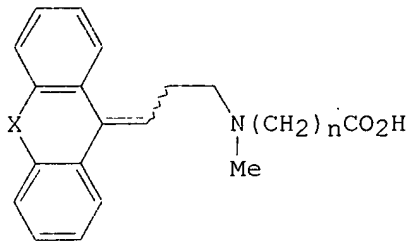
RN 158446-88-9 HCAPLUS
CN Glycine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 158446-92-5 HCAPLUS
CN Glycine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



L29 ANSWER 16 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1994:435305 HCAPLUS
DN 121:35305
TI Study on Zwitter-ionization of drugs. II. Synthesis and pharmacological activity of some N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methylamino- and N-[3-(6H-dibenz[b,e]oxepin-11-ylidene)propyl]-N-methylamino-alkanoic acid derivatives and related compounds
AU Muramatsu, Hiromi; Sawanishi, Hiroyuki; Iwasaki, Nobuhiko; Kakiuchi, Masato; Ohashi, Tetsuo; Kato, Hideo; Ito, Yasuo
CS Lab. Dev. Med., Hokuriku Univ., Kanazawa, 920-11, Japan
SO Chem. Pharm. Bull. (1993), 41(11), 1987-93
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
GI



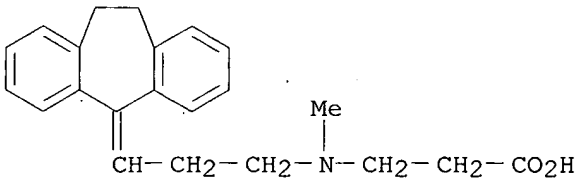
I

AB A series of N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methylamino- I (X = CH:CH, n = 1-5) and N-[3-(6H-dibenzo[b,e]oxepin-11-ylidene)propyl]-N-methylamino-alkanoic acid derivs. I (X = CH2O, n = 1-5) and related compds. I (X = CH2CH2, CH2S, O, S, n = 2) were synthesized and examd. for pharmacol. activities in vitro, i.e., inhibitory effect on monomaine [noradrenaline (NA) and 5-hydroxytryptamine (5-HT)] uptake, inhibitory effect on 5-HT, histamine-, acetylcholine- and NA-induced concn., and binding affinity for .alpha.2-adrenoceptor and dopamine D2-receptor. In vitro tests indicated that zwitter-ionization was capable of maintaining H1-antihistaminic activity while greatly reducing other pharmacol. activities. Further, I showed much stronger inhibitory effects on compd. 48/80-induced lethality in rats than did the corresponding N,N-dimethylamines. 3-[N-[3-(6H-dibenzo[b,e]oxpein-11-ylidene)propyl]-N-methylamino]-propionic acid, selected as a candidate antiallergic agent of a new type, equally potent in rats and guinea-pigs, exhibited strong inhibitory effects on 48 h homologous passive cutaneous anaphylaxis (PCA) in rats (ED50 = 0.019 mg/kg. p.o.) and on histamine-induced bronchoconstriction in anesthetized guinea-pigs (ED50 = 0.0067 mg/kg, p.o.).

IT **69436-99-3P 146623-41-8P 146623-42-9P 146623-43-0P 146623-44-1P 146623-45-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and antiallergic activity of)

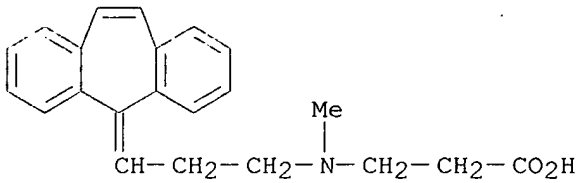
RN 69436-99-3 HCAPLUS

CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)

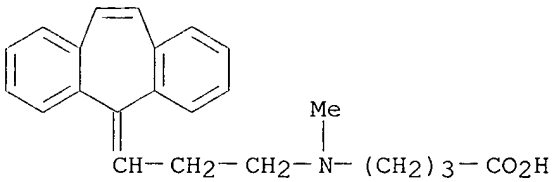


RN 146623-41-8 HCAPLUS

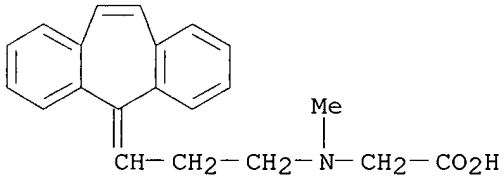
CN .beta.-Alanine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



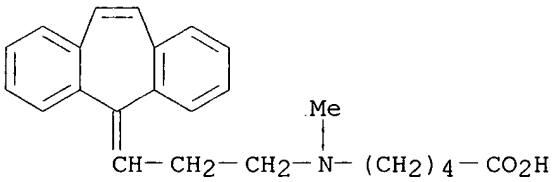
RN 146623-42-9 HCAPLUS
CN Butanoic acid, 4-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



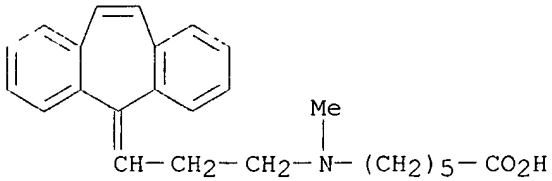
RN 146623-43-0 HCAPLUS
CN Glycine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



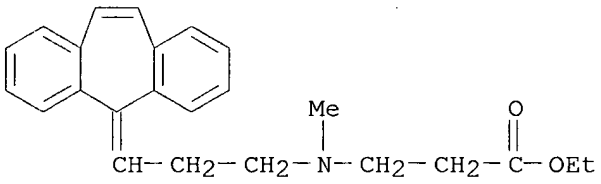
RN 146623-44-1 HCAPLUS
CN Pentanoic acid, 5-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



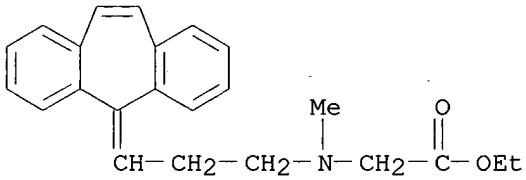
RN 146623-45-2 HCAPLUS
CN Hexanoic acid, 6-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



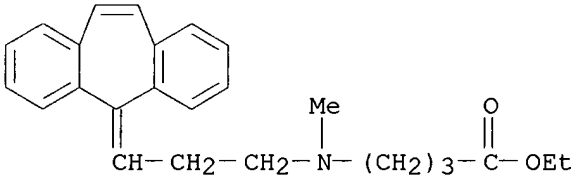
IT **146623-29-2P 146623-30-5P 146623-31-6P**
146623-32-7P 146623-33-8P 155588-55-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of alkenoic acid deriv.)
RN 146623-29-2 HCAPLUS
CN .beta.-Alanine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



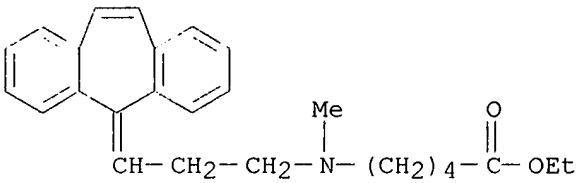
RN 146623-30-5 HCAPLUS
CN Glycine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



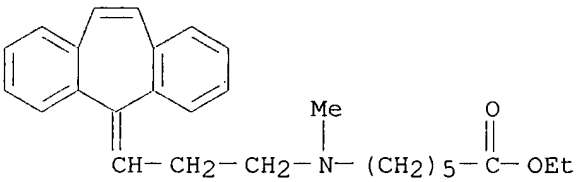
RN 146623-31-6 HCAPLUS
CN Butanoic acid, 4-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



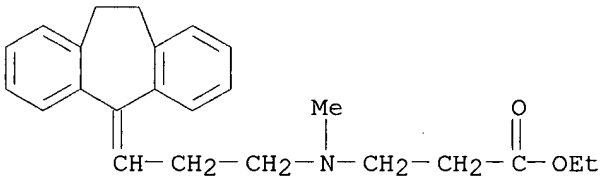
RN 146623-32-7 HCAPLUS
CN Pentanoic acid, 5-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 146623-33-8 HCAPLUS
CN Hexanoic acid, 6-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 155588-55-9 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 17 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1994:6782 HCAPLUS
DN 120:6782
TI Immunogenic composition against tricyclic antidepressant drugs
IN Blincko, Stuart J. F. E.
PA Therapeutic Antibodies, Inc., USA
SO U.S., 16 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

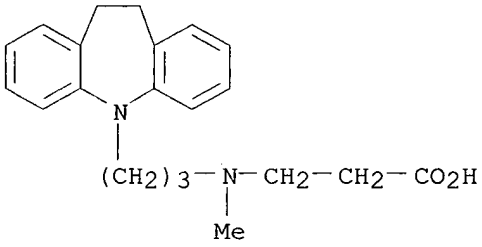
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5256409	A	19931026	US 1991-645799	19910125
PRAI GB 1990-1694		19900125		

AB An immunogenic compn. is disclosed for raising antisera to a tricyclic antidepressant drug. The immunogenic compn. comprises an immunol. active carrier protein to which is bound .gtoreq.2 types of hapten, each hapten comprising a drug mol., in which the drug mol. of one type of hapten is from the desimipramine/imipramine series of tricyclic antidepressants and the drug mol. of the 2nd type of hapten is from the nortriptyline/amitriptyline series of tricyclic antidepressants. The

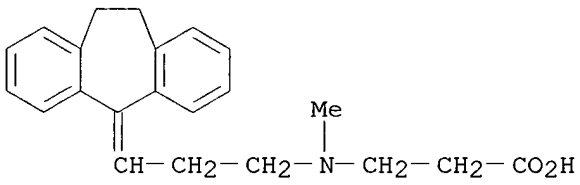
haptens may also have an optional bridging group. Also disclosed are a method for raising antisera using the immunogenic compn. and a method for alleviating an overdose of a tricyclic antidepressant comprising an effective amt. of the antisera raised to the immunogen. Thus, desimipramine Et carbonyl acid and nortriptyline Et carboxylic acid were prepd. and both were conjugated to hemocyanin. Immunoassay results demonstrated that the immunogens of the invention may be used to raise antisera in higher titer and with broader cross-reactivity properties than conventional immunogens.

IT **69241-80-1 69436-99-3 151779-02-1**
151779-03-2
RL: RCT (Reactant)
(Prepn. and reaction of, in immunogenic double conjugate prepn. for raising antisera to tricyclic antidepressants)

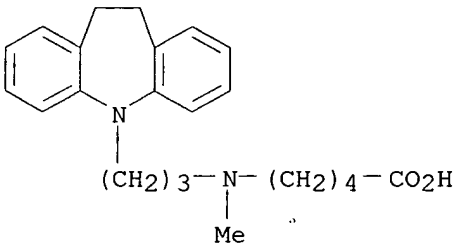
RN 69241-80-1 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)

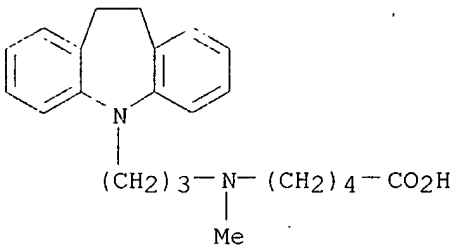


RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)

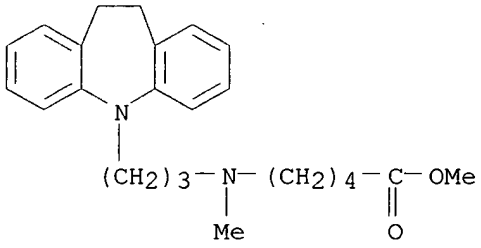


RN 151779-02-1 HCAPLUS
CN Pentanoic acid, 5-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



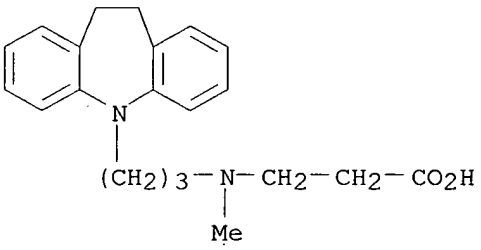


RN 151779-03-2 HCAPLUS
CN Pentanoic acid, 5-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-, methyl ester (9CI) (CA INDEX NAME)

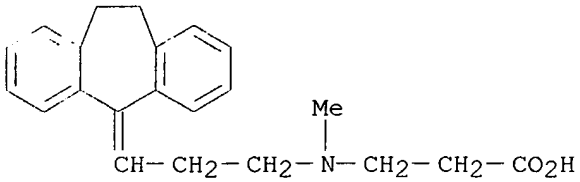


IT **69241-80-1DP**, conjugates with nortriptyline ethylcarbonyl-hemocyanin conjugates **69436-99-3DP**, conjugates with desipramine ethylacarbonyl-hemocyanin conjugates
RL: PREP (Preparation)
(prepn. of, for immunogen for raising antisera to tricyclic antidepressants)

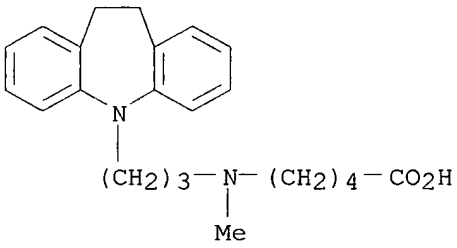
RN 69241-80-1 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



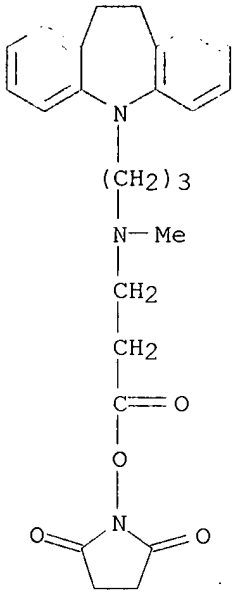
RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



IT **151779-02-1DP**, conjugates with desipramine ethylcarbonyl-hemocyanin conjugates
RL: PREP (Preparation)
(prepn. of, immunogen prepn. for raising antisera to tricyclic antidepressants in relation to)
RN 151779-02-1 HCAPLUS
CN Pentanoic acid, 5-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)

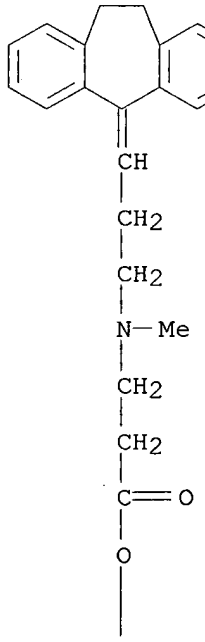


IT **151779-05-4P 151779-06-5P 151779-07-6P**
RL: PREP (Preparation)
(prepn. of, immunogenic double conjugate for raising antisera to tricyclic antidepressants in relation to)
RN 151779-05-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[3-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)

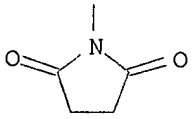


RN 151779-06-5 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[3-[[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-1-oxopropoxy]- (9CI) (CA INDEX NAME)

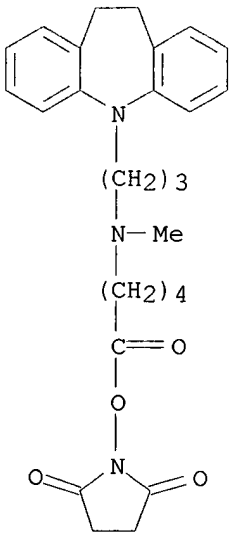
PAGE 1-A



PAGE 2-A



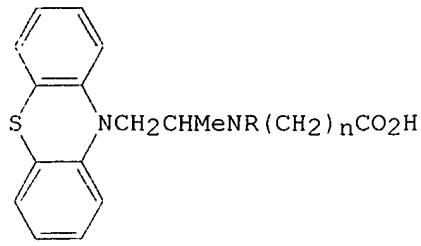
RN 151779-07-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[5-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-1-oxopentyl]oxy]- (9CI) (CA INDEX NAME)



L29 ANSWER 18 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1993:671182 HCAPLUS
DN 119:271182
TI Preparation of antihistaminic and antiallergic phenothiazines
IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Etsuchu, Eiichi; Saito, Keiko; Kurata, Sakae
PA Hokuriku Pharmaceutical, Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05163256	A2	19930629	JP 1991-351237	19911213

OS MARPAT 119:271182
GI



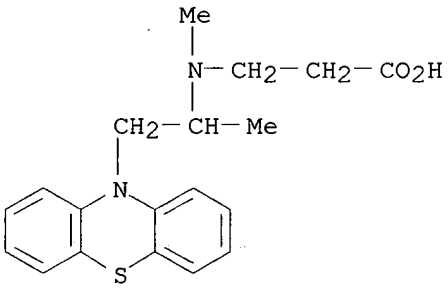
I

AB The title compds. I (R = lower alkyl; n = 1-5) and their salts, which show antihistaminic and antiallergic activities (no data), are prepd. A mixt. of 2.18 g 10-(2-methylaminopropyl)phenothiazine (prepn. given), 6.1 mL Et acrylate, and EtOH was refluxed for 90 min, mixed with NaOH, and refluxed for 2 h to give 2.74 g I (R = Me, n = 2).

IT **151340-16-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antihistaminic and antiallergic agent)

RN 151340-16-8 HCAPLUS

CN .beta.-Alanine, N-methyl-N-[1-methyl-2-(10H-phenothiazin-10-yl)ethyl]-(9CI) (CA INDEX NAME)



L29 ANSWER 19 OF 34 HCAPLUS COPYRIGHT 2002 ACS

AN 1993:649955 HCAPLUS

DN 119:249955

TI Tricyclic heterocyclic compounds as angiotensin II receptor antagonists

IN Ohshima, Etsuo; Kanai, Fumihiko; Sato, Hideyuki; Obase, Hiroyuki; Kumazawa, Toshiaki; Takahara, Shiho; Ohno, Tetsuji; Ishikawa, Tomoko; Yamada, Koji

PA Kyowa Hakko Kogyo Co., Ltd., Japan

SO Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW

DT Patent

LA English

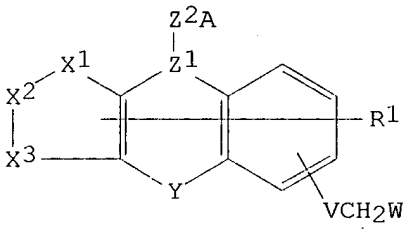
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 549352	A2	19930630	EP 1992-311777	19921224
	EP 549352	A3	19930728		
	EP 549352	B1	20000301		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 06228065	A2	19940816	JP 1992-344117	19921224

	JP 2526005	B2	19960821		
	AT 190058	E	20000315	AT 1992-311777	19921224
	ES 2142817	T3	20000501	ES 1992-311777	19921224
PRAI	JP 1991-347294	A	19911227		

OS MARPAT 119:249955

GI



I

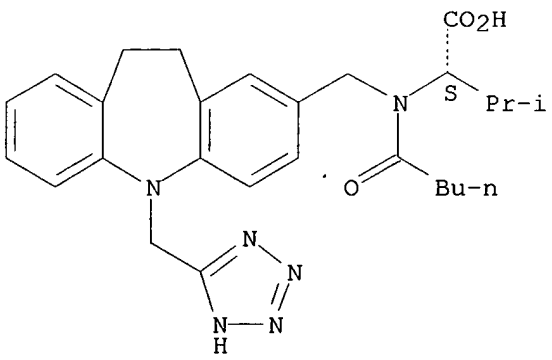
AB The title compds. I [A = CN, CO2H, tetrazolyl, (un)substituted Ph; R1 = H, halogen, C1-6 alkyl; V = (CH2)m; m = 0-2; W = (un)substituted imidazolo, (un)substituted acylamino, (un)substituted phenylamino or pyridylamino; X1-X2-X3 = CH:CHCH:CH, SCH:CH, CH:CHS; Y = CH2, single bond, O, S, CH2O, OCH2, CH2S, SCH2, CH2CH2, CH:CH; Z1-Z2 = C:CH, CHCH2, CHCH(CO2H), N(CH2)n; n = 1-3], useful in the treatment of hypertension, are prepd. and I-contg. pharmaceutical formulations presenced. Thus, 2-(5,7-dimethyl-2-cyclopropyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl-5-(1H-tetrazol-5-yl)methyl-5H-10,11-dihydrodibenz[b,f]azepine K salt (II) was, prepd. from 5,7-dimethyl-2-cyclopropyl-3H-phenimidazo[4,5-b]pyridine. II demonstrated inhibition rate [1-[(binding amt. in the presence of a test compd.)-(nonspecific binding amt.)/(total binding amt.)-(nonspecific binding amt.)]] x 100] against angiotensin II receptors from bovine adrenal cortex of 97%.

IT **150802-67-8P 150802-75-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and angiotensin II receptor antagonists activity of)

RN 150802-67-8 HCAPLUS

CN L-Valine, N-[[10,11-dihydro-5-(1H-tetrazol-5-ylmethyl)-5H-dibenz[b,f]azepin-2-yl]methyl]-N-(1-oxopentyl)- (9CI) (CA INDEX NAME)

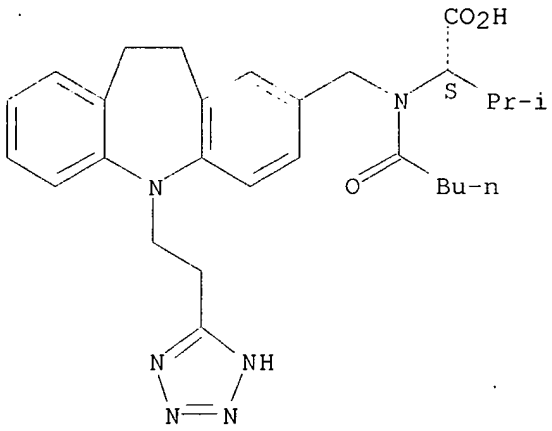
Absolute stereochemistry.



RN 150802-75-8 HCAPLUS

CN L-Valine, N-[[10,11-dihydro-5-[2-(1H-tetrazol-5-yl)ethyl]-5H-dibenz[b,f]azepin-2-yl]methyl]-N-(1-oxopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

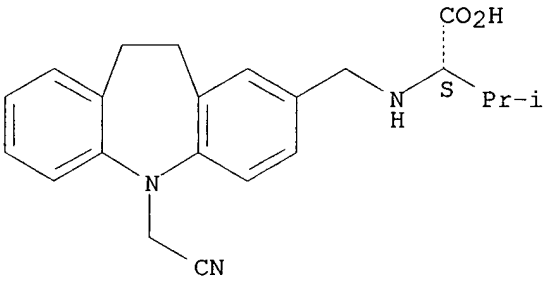


IT **150802-69-0P 150802-70-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of angiotensin II receptor antagonists)

RN 150802-69-0 HCAPLUS

CN L-Valine, N-[[5-(cyanomethyl)-10,11-dihydro-5H-dibenz[b,f]azepin-2-yl]methyl]- (9CI) (CA INDEX NAME)

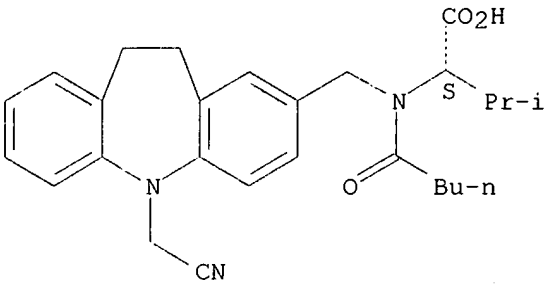
Absolute stereochemistry.



RN 150802-70-3 HCAPLUS

CN L-Valine, N-[[5-(cyanomethyl)-10,11-dihydro-5H-dibenz[b,f]azepin-2-yl]methyl]-N-(1-oxopentyl)- (9CI) (CA INDEX NAME)

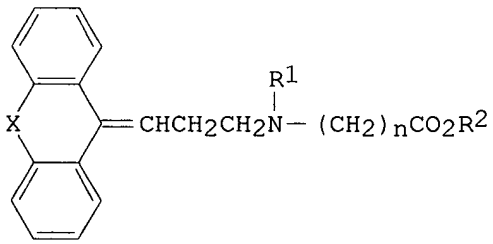
Absolute stereochemistry.



L29 ANSWER 20 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1993:192291 HCAPLUS
DN 118:192291
TI Preparation of dibenzopyran analogs as allergy inhibitors.
IN Sawanishi, Hiroyuki; Ito, Yasuo; Kato, Hideo; Koshinaka, Eiichi; Ogawa, Nobuo; Morikawa, Kouji
PA Hokuriku Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9217440	A1	19921015	WO 1992-JP365	19920326
	W: AU, CA, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	JP 05078292	A2	19930330	JP 1992-75587	19920227
	AU 9214469	A1	19921102	AU 1992-14469	19920326
	EP 589038	A1	19940330	EP 1992-907619	19920326
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
	US 5432192	A	19950711	US 1993-122603	19931001
PRAI	JP 1991-99775		19910405		
	JP 1991-144107		19910521		
	JP 1992-75587		19920227		
	WO 1992-JP365		19920326		

OS MARPAT 118:192291
GI



I

AB The title compds. [I; X = CH:CH, CH2O, O; R1 = alkyl; R2 = H, alkyl; n = 1-5 integer] are prepd. E.g., a mixt. of 5-[3-(methylamino)propylidene]-

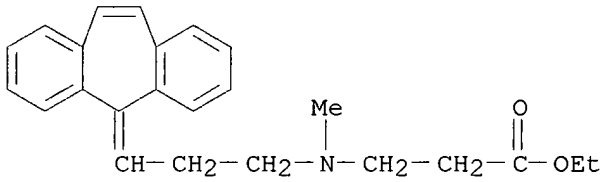
5H-dibenzo[a,d]cycloheptene and Et acrylate in EtOH was refluxed for 2 H to give I [R1 = Me, R2 = Et, n = 2, X = CH:CH]. In an in vitro study using isolate rat ileum I [R1, n, X the same as above; R2 = H] (also prepd.) had an -log KB value of 8.16 against histamine.

IT **146623-29-2P 146623-30-5P 146623-31-6P 146623-32-7P 146623-33-8P 146623-41-8P 146623-42-9P 146623-43-0P 146623-44-1P 146623-45-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as allergy inhibitor)

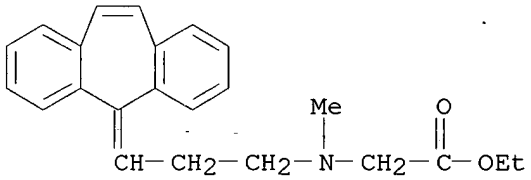
RN 146623-29-2 HCAPLUS

CN .beta.-Alanine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



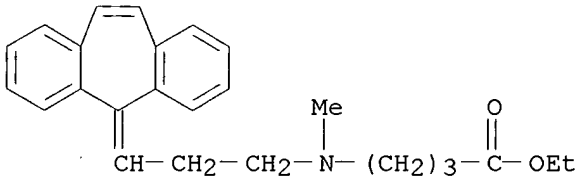
RN 146623-30-5 HCAPLUS

CN Glycine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



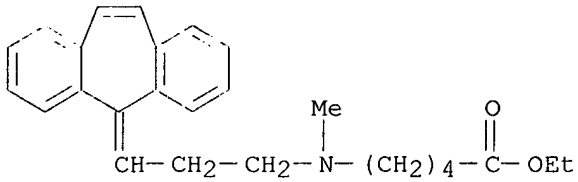
RN 146623-31-6 HCAPLUS

CN Butanoic acid, 4-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)

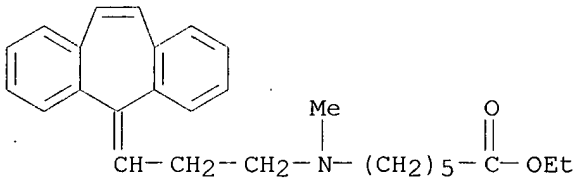


RN 146623-32-7 HCAPLUS

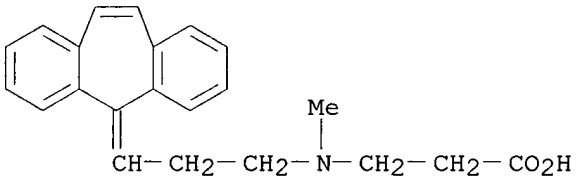
CN Pentanoic acid, 5-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



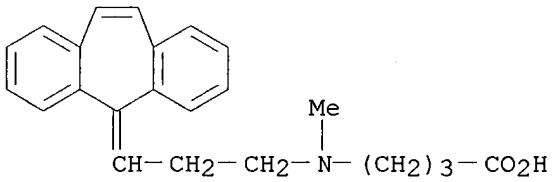
RN 146623-33-8 HCAPLUS
CN Hexanoic acid, 6-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)



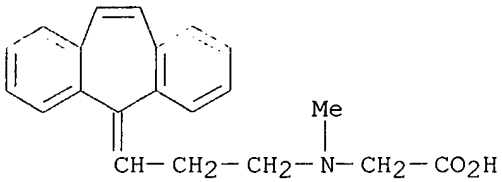
RN 146623-41-8 HCAPLUS
CN .beta.-Alanine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



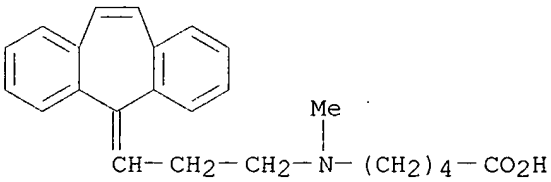
RN 146623-42-9 HCAPLUS
CN Butanoic acid, 4-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)



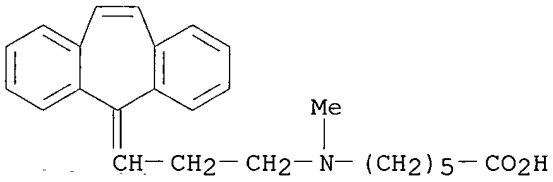
RN 146623-43-0 HCAPLUS
CN Glycine, N-[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 146623-44-1 HCAPLUS
CN Pentanoic acid, 5-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)

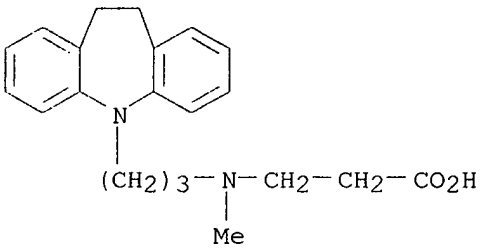


RN 146623-45-2 HCAPLUS
CN Hexanoic acid, 6-[[3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]methylamino]- (9CI) (CA INDEX NAME)

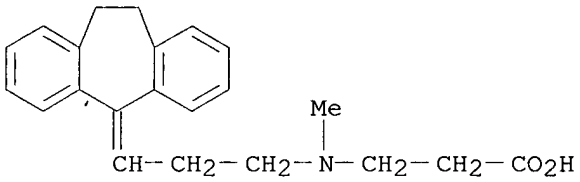


L29 ANSWER 21 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1990:441284 HCAPLUS
DN 113:41284
TI A synthesis of N-substituted .beta.-alanines: Michael addition of amines to trimethylsilyl acrylate
AU Kwiatkowski, Stefan; Jeganathan, Azhwarsamy; Tobin, Thomas; Watt, David S.
CS Maxwell H. Gluck Equine Res. Cent., Univ. Kentucky, Lexington, KY, 40506, USA
SO Synthesis (1989), (12), 946-9
CODEN: SYNTBF; ISSN: 0039-7881
DT Journal
LA English
OS CASREACT 113:41284
AB Michael addn. of primary and secondary amines to H2C:CHCO2SiMe3 gave .beta.-(alkylamino)- and .beta.-(dialkylamino)propanoic acids in 37-99% yields. This method was used to functionalize a wide variety of biol. active amines.
IT **69241-80-1P 69436-99-3P 128013-78-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 69241-80-1 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-

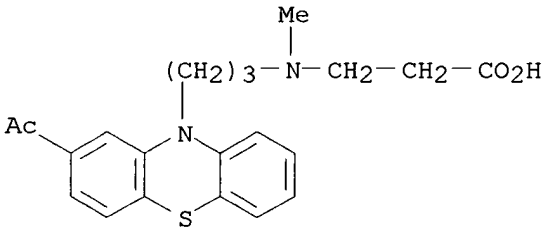
methyl- (9CI) (CA INDEX NAME)



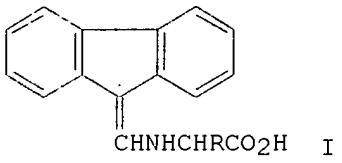
RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 128013-78-5 HCAPLUS
CN .beta.-Alanine, N-[3-(2-acetyl-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)

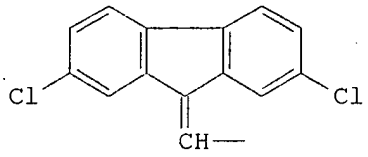


L29 ANSWER 22 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1989:515735 HCAPLUS
DN 111:115735
TI Investigation of the reaction between amino acids or amino acid esters and 9-formylfluorene and its equivalents. Possible utility of the derived enamines as amino group protectants
AU Carpino, Louis A.; Chao, Hann Guang; Tien, Jien Heh
CS Dep. Chem., Univ. Massachusetts, Amherst, MA, 01003, USA
SO J. Org. Chem. (1989), 54(18), 4302-13
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 111:115735
GI



I

DC-FM-bar=

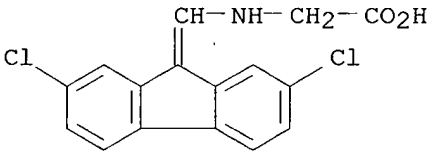


AB Treatment of 9-(hydroxymethylene)fluorene/9-formylfluorene (storable as the hemiacetal with methanol) with amino acids and amino acid esters yields the corresponding enamines, which may be considered to be hydrocarbon analogs of N-formyl amino acid derivs. Attempted coupling of the free acids I (R = amino acid side chain) with amino acid esters failed, suggesting insufficient redn. in basicity of the amino group due to the enamine residue. The introduction of electron-withdrawing substituents into the fluorene ring decreases the basicity sufficiently to allow normal peptide coupling reactions, as for example with analogs derived from 2,7-dichloro-9 hydroxymethylene 9H-fluorene. Thus, DC-FM-bar-Phe-OH was coupled with H-Leu-OMe by DCC to give dipeptide DC-FM-bar-Phe-Leu-OMe. The DC-FM-bar group could be removed by catalytic transfer hydrogenolysis. Mild acid hydrolysis represents a second general deblocking technique for the FM-bar function. It was demonstrated in a model study with the highly sensitive H2NCHPhCO2H that the FM-bar protecting group was less prone to cause racemization than the benzyloxycarbonyl function. Leucine-enkephalin was prepd. using .alpha.-DC-FM-bar protection along with tert-butyl-based side chain protecting groups.

IT **122236-84-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tripeptide tert-Bu ester)

RN 122236-84-4 HCAPLUS

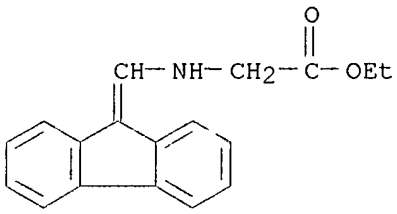
CN Glycine, N-[(2,7-dichloro-9H-fluoren-9-ylidene)methyl]- (9CI) (CA INDEX NAME)



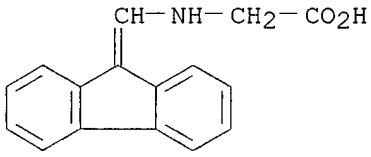
IT **122236-82-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)

RN 122236-82-2 HCAPLUS

CN Glycine, N-(9H-fluoren-9-ylidenemethyl)-, ethyl ester (9CI) (CA INDEX NAME)

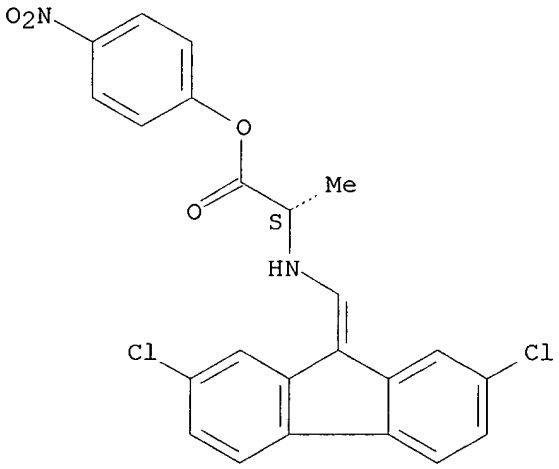


IT **122236-83-3P 122236-93-5P 122236-95-7P**
122237-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 122236-83-3 HCAPLUS
CN Glycine, N-(9H-fluoren-9-ylidenemethyl)- (9CI) (CA INDEX NAME)



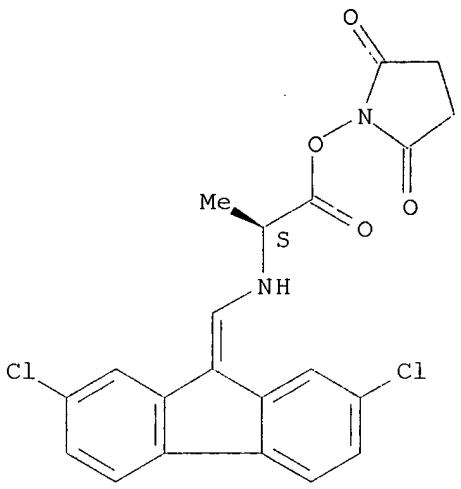
RN 122236-93-5 HCAPLUS
CN L-Alanine, N-[(2,7-dichloro-9H-fluoren-9-ylidene)methyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

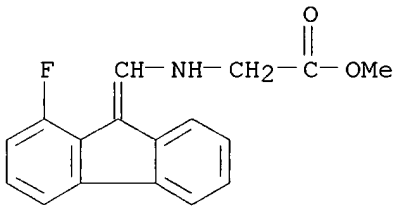


RN 122236-95-7 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[2-[[(2,7-dichloro-9H-fluoren-9-ylidene)methyl]amino]-1-oxopropoxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

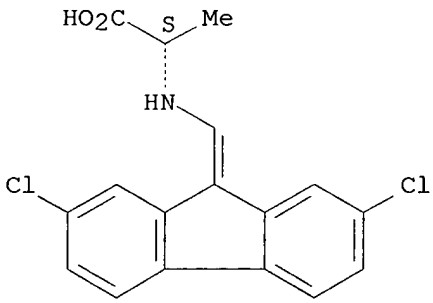


RN 122237-08-5 HCAPLUS
CN Glycine, N-[(1-fluoro-9H-fluoren-9-ylidene)methyl]-, methyl ester (9CI) (CA INDEX NAME)



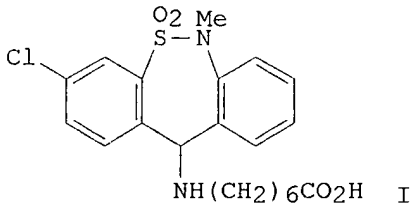
IT **122236-85-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., esterification, and peptide coupling of)
RN 122236-85-5 HCAPLUS
CN L-Alanine, N-[(2,7-dichloro-9H-fluoren-9-ylidene)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



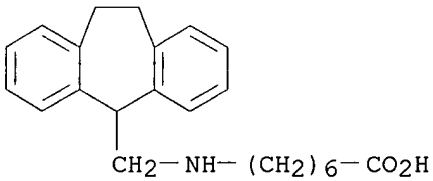
L29 ANSWER 23 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1989:50715 HCAPLUS

DN 110:50715
TI Structure-activity relationships of tricyclic antidepressants, with special reference to tianeptine
AU Labrid, C.; Moleyre, J.; Poignant, J. C.; Malen, C.; Mocaer, E.; Kamoun, A.
CS Inst. Rech. Int. Serv., Neuilly-sur-Seine, 92200, Fr.
SO Clin. Neuropharmacol. (1988), 11(Suppl. 2), S21-S31
CODEN: CLNEDB; ISSN: 0362-5664
DT Journal
LA English
GI



I

AB The authors studied the structure-activity relationships of tianeptine (I) and its derivs. exhibiting reserpine-induced ptosis reversal potency in the mouse. Tianeptine is an antidepressant characterized by a 3-chlorodibenzothiazepin nucleus and an aminoheptanoic side chain. The results indicate highly specific structural requirements for the tianeptine-like series. In order to be active, compds. must have an aminocarboxylic chain (with an optimal length of 6 methylene links), a tricyclic system with an electron-donor heteroatom in position 5, and an arom. substitution with a moderate electron-acceptor atom in position 3. These specificities in the tianeptine series are in sharp contrast with the lack of specific requirements that characterize the classical tricyclic series.
IT **118409-35-1**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antidepressant activity of, structure in relation to)
RN 118409-35-1 HCAPLUS
CN Heptanoic acid, 7-[[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)methyl]amino]- (9CI) (CA INDEX NAME)

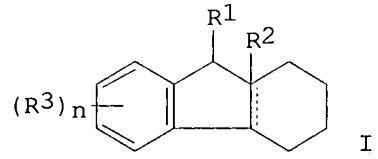


L29 ANSWER 24 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1988:492529 HCAPLUS
DN 109:92529
TI Hydrofluorene derivatives for the treatment of hypoxic conditions, their

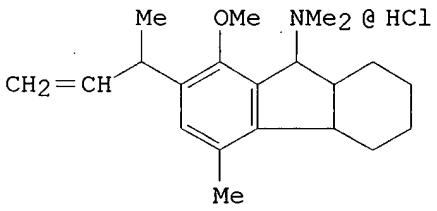
pharmaceutical formulations, and a process for their preparation
IN Oshiro, Yasuo; Tanaka, Tatsuyoshi; Sakurai, Yoji; Sato, Seiji
PA Otsuka Pharmaceutical Co., Ltd., Japan
SO Eur. Pat. Appl., 142 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 267024	A2	19880511	EP 1987-309771	19871104
	EP 267024	A3	19890315		
	EP 267024	B1	19910502		
	R: CH, DE, ES, FR, GB, IT, LI, NL, SE				
	JP 63253055	A2	19881020	JP 1987-277875	19871102
	JP 2568416	B2	19970108		
	DK 8705753	A	19880505	DK 1987-5753	19871103
	CN 87107628	A	19880608	CN 1987-107628	19871104
	CN 1022685	B	19931110		
	ES 2031911	T3	19930101	ES 1987-309771	19871104
	US 5017724	A	19910521	US 1990-532341	19900604
PRAI	JP 1986-263561		19861104		
	US 1987-116698		19871104		

OS MARPAT 109:92529
GI



I

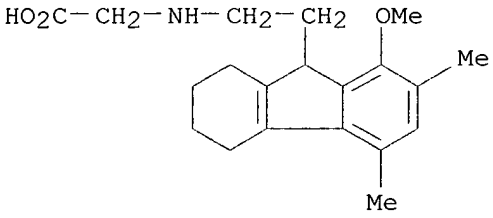


II

AB Title derivs. I [R1 = :NR4 NR5R6, (un)substituted aminoalkyl; R2 = H, alkoxy, alkyl; R3 = H, alkyl, halo, alkenyl, phenylalkenyl, NO2, cycloalkylalkyl, phenylalkyl, alkoxy, alkylthio, alkylthioalkyl, cyano alkanoyl, CO2H, OH, (alkyl)aminoalkyl, cycloalkyl, cycloalkenyl, alkyl- or alkanoylamino; R4 = OH, alkyl; R5,R6 = H, cycloalkyl, alkenyl, alkynyl, Ph, phenylalkyl, pyridylcarbonyl, (un)substituted alkyl, alkanoyl, piperidinyl, aminoalkanoyl; NR5R6 = satd. 5- or 6-membered heterocyclyl with optional oxo substituent; n = 0-3; dotted line = optional bond] are prepd. as agents for treating cerebral conditions related to hypoxia and/or lowered acetylcholinergic nervous system function. Methylation of 7-(1-methyl-2-propenyl)-8-hydroxy-5-methyl-9-methylamino-1,2,3,4,4a,9a-hexahydrofluorene using NaH/MeI in DMF gave, after acidification, (dimethylamino)methoxy(methylpropenyl)methylhexahydrofluorene

hydrochloride II. At 100 mg/kg orally in KCN-poisoned mice, II extended survival times by 27%.

IT **115807-30-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for treatment of hypoxia and brain disorders)
RN 115807-30-2 HCAPLUS
CN Glycine, N-[2-(2,3,4,9-tetrahydro-8-methoxy-5,7-dimethyl-1H-fluoren-9-yl)ethyl]- (9CI) (CA INDEX NAME)

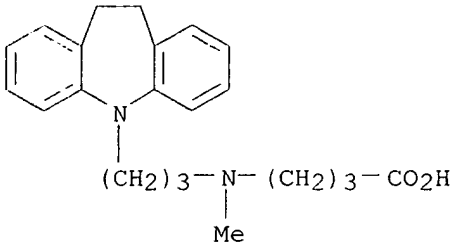


L29 ANSWER 25 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1987:113537 HCAPLUS
DN 106:113537
TI Preparation of tricyclic antidepressant conjugates with proteins and their uses as immunogens for antibody production for immunoassay
IN Collins, Christine G.; Pirio, Marcel R.; Singh, Prithipal
PA Syntex (U.S.A.), Inc., USA
SO U.S., 10 pp. Cont.-in-part of U.S. Ser. No. 518,905, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

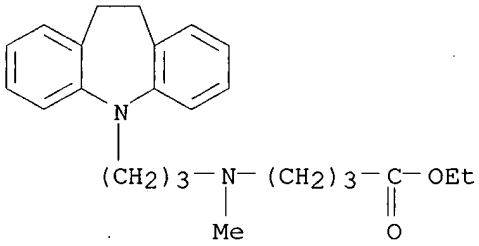
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4629691	A	19861216	US 1983-522887	19830812
	US 4772697	A	19880920	US 1986-898559	19860821
PRAI	US 1983-518905		19830901		
	US 1983-522887		19830812		

AB Tricyclic antidepressant derivs. are prepd. in which the methylaminopropyl side chain is functionalized for conjugation to antigenic compds., particularly poly(amino acids), and enzymes. The antigenic conjugate is used as an immunogen. The resultant antibodies are used with the enzyme conjugate in immunoassays for the detn. of tricyclic antidepressants in serum or other body fluids. Desmethylimipramine was alkylated with ethyl-4-bromobutyrate. The product was sapond., conjugated with bovine serum albumin, and used as an immunogen. N-carboglycylpropyldesmethylimipramine conjugated with glucose-6-phosphate dehydrogenase and antibodies to the immunogen were used in a homogeneous enzyme immunoassay of amitriptyline, nortriptyline, imipramine, and desmethylimipramine.

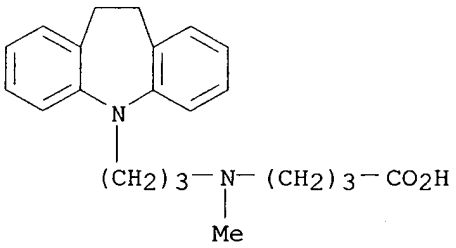
IT **107220-00-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conjugation to bovine serum albumin)
RN 107220-00-8 HCAPLUS
CN Butanoic acid, 4-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



IT **107220-01-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
RN 107220-01-9 HCAPLUS
CN Butanoic acid, 4-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]-, ethyl ester (9CI) (CA INDEX NAME)

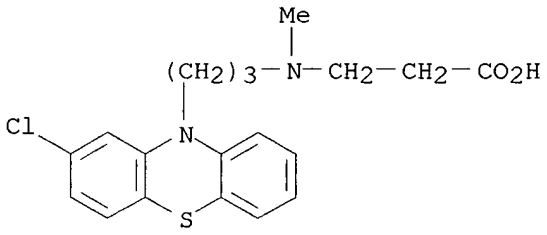


IT **107220-00-8DP**, serum albumin or globulin conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as immunogen)
RN 107220-00-8 HCAPLUS
CN Butanoic acid, 4-[[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]methylamino]- (9CI) (CA INDEX NAME)



L29 ANSWER 26 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1986:471970 HCAPLUS
DN 105:71970
TI Preparation of two chlorpromazine antigens
AU Zhu, Jianhua; Bai, Shikang
CS Nucl. Med. Inst., Shanghai 1st Med. Coll., Shanghai, Peop. Rep. China

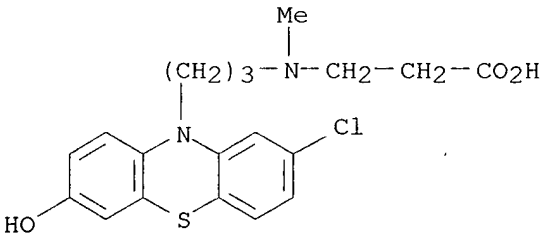
SO Hejishu (1985), (2), 50-2
CODEN: NUTEDL
DT Journal
LA Chinese
AB Two 7-(3-carboxypropionyl)chloropromazine-bovine serum albumin conjugates (with drug/albumin mol. ratios of 5 and 31) and 1 N-(2-carboxyethyl)demethylchloropromazine-bovine serum albumin conjugate (with mol. ratio 33) were prepd. The antiserum titer in rabbits immunized with the conjugates with mol. ratios 31 and 33 was 28,000 and 12,000, resp.; these 2 conjugates are useful chlorpromazine [50-53-3] antiserum-inducing agents for radioimmunoassay. The conjugate with mol. ratio 5 produced a very low titer of antiserum and had no practical use in radioimmunoassay.
IT **69436-77-7D**, conjugates with bovine serum albumin
RL: BIOL (Biological study)
(antiserum to, for chlorpromazine radioimmunoassay)
RN 69436-77-7 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



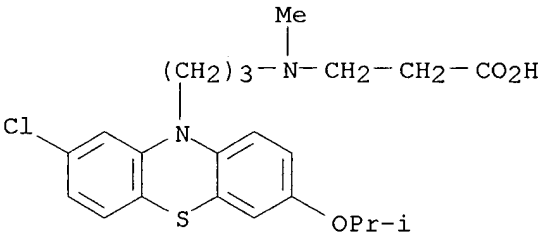
L29 ANSWER 27 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1985:498221 HCAPLUS
DN 103:98221
TI A comparison of two radioimmunoassays for 7-hydroxychlorpromazine: rabbit polyclonal antibodies vs. mouse monoclonal antibodies
AU Yeung, P. K. F.; McKay, G.; Ramshaw, I. A.; Hubbard, J. W.; Midha, K. K.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.
SO J. Pharmacol. Exp. Ther. (1985), 233(3), 816-22
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
AB Two radioimmunoassays (RIAs) were developed for 7-hydroxychlorpromazine (7-OHCPZ) [2095-62-7], a pharmacol. active chlorpromazine (CPZ) metabolite. One of the RIAs used polyclonal antibodies produced in rabbits immunized with a 7-OHCPZ-protein conjugate, which was prepd. by coupling 7-hydroxy-N-(2-carboxyethyl)desmethylchlorpromazine to bovine serum albumin by a mixed anhydride method (90% yield). The other RIA was based on mouse monoclonal antibodies produced by hybridomas against the same conjugate. The mouse monoclonal antibodies were considerably more specific than the rabbit polyclonal antibodies. There was little interference with the measurement of 7-OHCPZ by RIA based on mouse monoclonal antibodies even when the samples were spiked with 7-OHCPZ in the presence of five times excess of CPZ and two major metabolites, CPZ sulfoxide and CPZ-N-oxide. By contrast, there was a significant increase in the apparent concn. of 7-OHCPZ when the same samples were assayed by RIA based on polyclonal antibodies. The RIA based on mouse monoclonal

antibodies was applied, together with an RIA for CPZ to det. the concns. of 7-OHCPZ and CPZ in plasma samples from 2 healthy volunteers after they had received a single 50 mg oral dose of CPZ. Plasma 7-OHCPZ concns., measured up to 24 h after a single dose of CPZ, are reported.

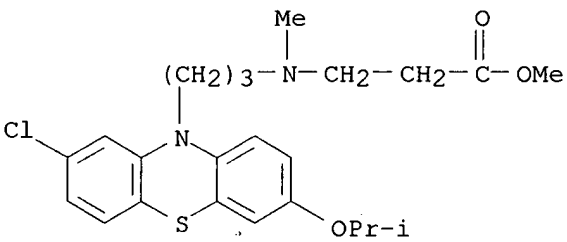
IT **97777-76-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conjugation with serum albumin)
RN 97777-76-9 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-7-hydroxy-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



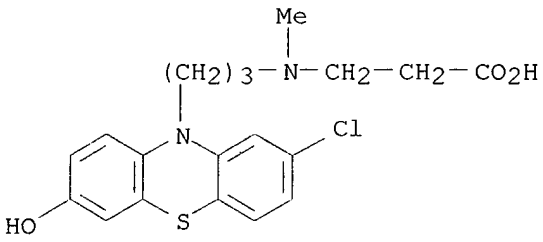
IT **97777-75-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of)
RN 97777-75-8 HCAPLUS
CN .beta.-Alanine, N-[3-[2-chloro-7-(1-methylethoxy)-10H-phenothiazin-10-yl]propyl]-N-methyl- (9CI) (CA INDEX NAME)



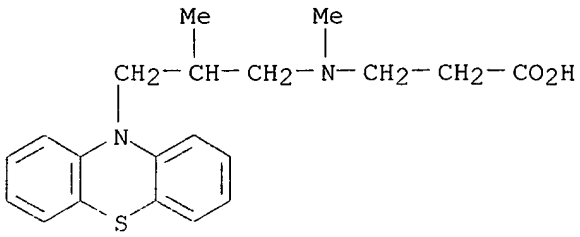
IT **97777-74-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 97777-74-7 HCAPLUS
CN .beta.-Alanine, N-[3-[2-chloro-7-(1-methylethoxy)-10H-phenothiazin-10-yl]propyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



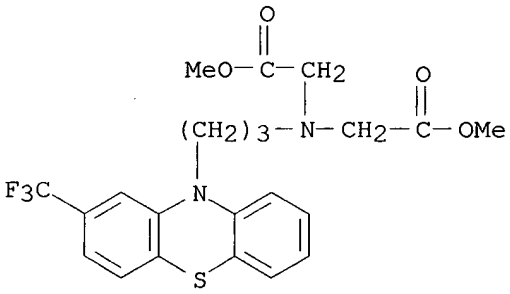
IT **97777-76-9DP**, serum conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for radioimmunoassay of hydroxychlorpromazine in blood)
RN 97777-76-9 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-7-hydroxy-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



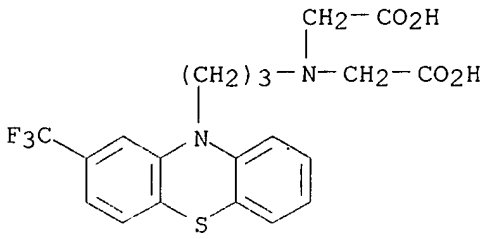
L29 ANSWER 28 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1985:17004 HCAPLUS
DN 102:17004
TI Radioimmunoassay for trimeprazine in human plasma
AU McKay, G.; Rauw, G. A. J.; Stonkus, M. D.; Dulos, R. A.; Gedir, R. G.; Hawes, E. M.; Midha, Kamal K.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.
SO J. Pharmacol. Methods (1984), 12(3), 203-11
CODEN: JPMED9; ISSN: 0160-5402
DT Journal
LA English
AB Antisera to trimeprazine [84-96-8] were raised in rabbits to an immunogen synthesized by covalent linkage of bovine serum albumin to N-(2-carboxyethyl)dexmethyltrimeprazine. By use of an antiserum, a radioimmunoassay for trimeprazine was developed that is able to quantitate 0.38 ng/mL in a 200 .mu.L plasma sample with a coeff. of variation of approx. 12%. The antiserum did not cross-react with the supposedly pharmacol. inactive metabolite trimeprazine sulfoxide [10071-07-5]; however, the cross-reactivity with the supposedly active metabolite N-desmethyltrimeprazine [22732-04-3] is significant (49%). The radioimmunoassay was able to measure the drug and(or) N-desalkyl metabolites in plasma samples obtained as late as 24 h following administration of a single oral dose (10 mg) of trimeprazine tartrate [4330-99-8]. Anal. of the same plasma samples by HPLC procedure gave values much lower than those obtained by the radioimmunoassay, indicating that the N-desalkyl metabolites are produced after trimeprazine oral administration.
IT **94015-99-3DP**, albumin conjugates
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and antibodies to, for trimeprazine radioimmunoassay)
RN 94015-99-3 HCAPLUS
CN .beta.-Alanine, N-methyl-N-[2-methyl-3-(10H-phenothiazin-10-yl)propyl]- (9CI) (CA INDEX NAME)



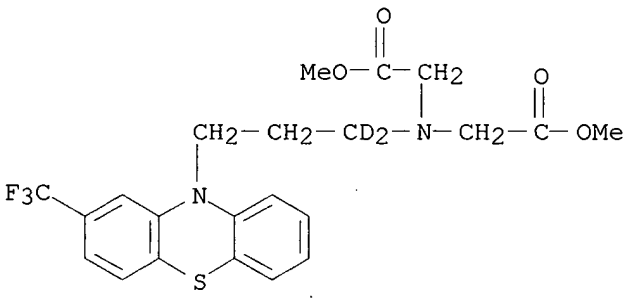
L29 ANSWER 29 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1984:156567 HCAPLUS
DN 100:156567
TI Synthesis of deuterium-labeled fluphenazine
AU Shetty, H. Umesha; Hawes, Edward M.; Midha, Kamal K.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.
SO J. Pharm. Sci. (1984), 73(1), 87-90
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal
LA English
AB The propylpiperazine side chain of fluphenazine has been labeled with 2, 4, and 6 D atoms by LiAlD4 redn. of the appropriate ester or imide. The .gamma.-C of the Pr group was labeled with 2 D atoms by redn. of 10-(2-methoxycarbonylethyl)-2-trifluoromethyl-10H-phenothiazine, while 4 D atoms were incorporated into the piperazine ring by redn. of 10-[3-(3,5-dioxo-1-piperazinyl)propyl]-2-trifluoromethyl-10H-phenothiazine. The latter redn. gave the d4 labeled N-de(hydroxyethyl) metabolite of fluphenazine.
IT **89507-44-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 89507-44-8 HCAPLUS
CN Glycine, N-(2-methoxy-2-oxoethyl)-N-[3-[2-(trifluoromethyl)-10H-phenothiazin-10-yl]propyl]-, methyl ester (9CI) (CA INDEX NAME)



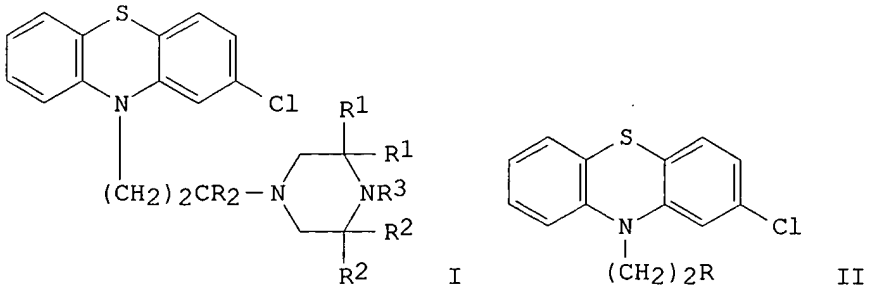
IT **89507-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with urea)
RN 89507-46-0 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-[3-[2-(trifluoromethyl)-10H-phenothiazin-10-yl]propyl]- (9CI) (CA INDEX NAME)



IT **89507-45-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., hydrolysis, and reaction of, with urea)
RN 89507-45-9 HCAPLUS
CN Glycine, N-(2-methoxy-2-oxoethyl)-N-[3-[2-(trifluoromethyl)-10H-phenothiazin-10-yl]propyl-1,1-d2]-, methyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 30 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1983:612478 HCAPLUS
DN 99:212478
TI Synthesis of deuterium-labeled perphenazine
AU Hawes, E. M.; Gurnsey, T. S.; Shetty, H. U.; Midha, K. K.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, S7N 0W0, Can.
SO J. Labelled Compd. Radiopharm. (1983), 20(6), 757-69
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
OS CASREACT 99:212478
GI



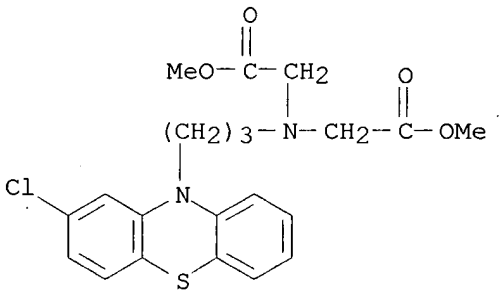
I

II

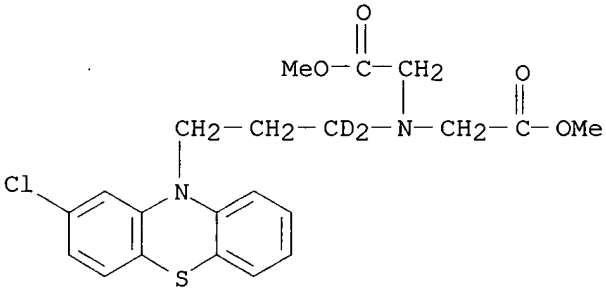
AB Perphenazines I [R = H, D, R1 = R2 = H, R3 = (CH2)2OH] were prepd. from ester II (R = CO2Me) by redn. with LiAlH4 or LiAlD4 followed by bromination and condensation with (2-hydroxyethyl)piperazine. Condensation of II (R = CH2Br, CD2Br) with HN(CH2CO2Me)2 followed by hydrolysis and cyclocondensation with urea gave imides I (R = H, D, R12 = R22 = O, R3 = H) (III). Redn. of III with LiAlD4 gave I (R = H, D, R1 = R2 = D, R3 = H); condensation of these compds. with Br(CH2)2OH gave I [R = H, D, R1 = R2 = D, R3 = (CH2)2OH].

IT **87893-70-7P 87893-71-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclocondensation reaction of, with urea, chloro[(dioxopiperazinyl)propyl]phenothiazine by)

RN 87893-70-7 HCAPLUS
CN Glycine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)

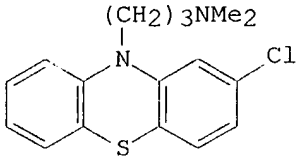


RN 87893-71-8 HCAPLUS
CN Glycine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl-1,1-d2]-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 31 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1983:587024 HCAPLUS
DN 99:187024
TI A study of the kinetics of chlorpromazine sulfoxide by a specific radioimmunoassay after a single oral dose of chlorpromazine in healthy volunteers
AU Yeung, P. K. F.; Hubbard, J. W.; Cooper, J. K.; Midha, K. K.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.
SO J. Pharmacol. Exp. Ther. (1983), 226(3), 833-8

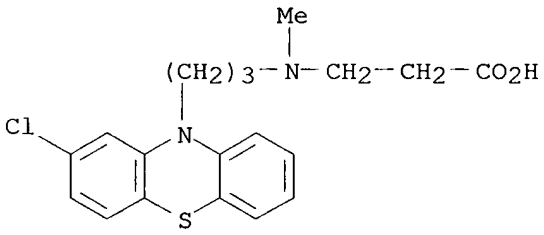
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
GI



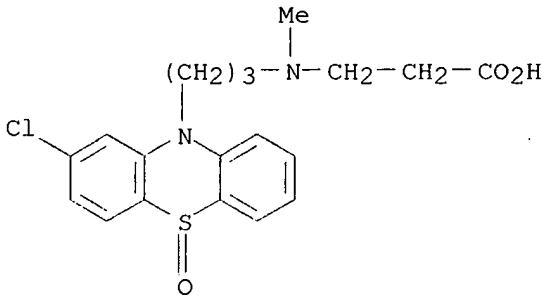
I

AB Antibody specific for chlorpromazine sulfoxide (CPZSO) [969-99-3] was produced in rabbits immunized with a hapten-bovine serum albumin conjugate, which was prepd. by linking the 10-alkyl side chain of CPZSO to the protein mol. via a 2-carbon bridge. A simple radioimmunoassay was developed which can measure < 20 pg of CPZSO in plasma. The assay had adequate specificity so that isolation of CPZSO was unnecessary. It was used together with a previously developed chlorpromazine (CPZ)(I) [50-53-3] radioimmunoassay to det. the concns. of CPZ and CPZSO in plasma samples from 5 healthy volunteers after they had received a single 50-mg oral dose of CPZ. A significant portion of CPZ was metabolized to CPZSO during presystemic absorption. There are, however, differences to those previously reported in the plasma concn. ratios of CPZSO to CPZ. The possible reasons for these differences are discussed.

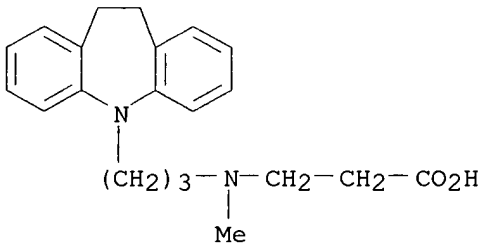
IT **69436-77-7**
RL: RCT (Reactant)
(oxidn. of)
RN 69436-77-7 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



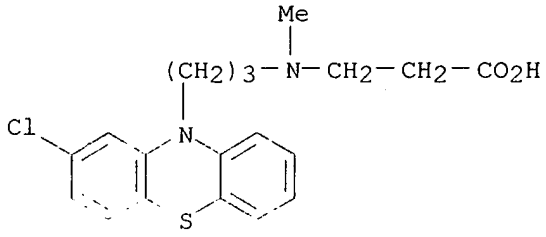
IT **87687-18-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with serum albumins of)
RN 87687-18-1 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-5-oxido-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



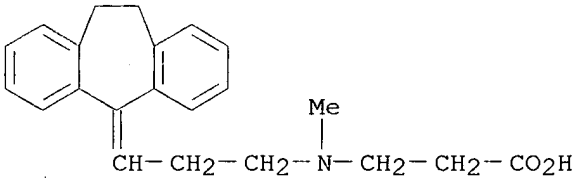
L29 ANSWER 32 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1981:479435 HCAPLUS
DN 95:79435
TI The mass spectral fragmentation of some carboxylic acid derivatives of psychotropic drugs
AU Hubbard, J. W.; Midha, K. K.; Cooper, J. K.; Charette, C.
CS Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, R3T 2N2, Can.
SO Can. J. Pharm. Sci. (1981), 15(4), 89-93
CODEN: CNJPAZ; ISSN: 0008-4190
DT Journal
LA English
AB The fragmentation pathways of some .beta.-amino-carboxylic acid and .beta.-carbamoyl-carboxylic acid derivs. of psychotropic drugs under electron impact, were examd. under a variety of mass spectral conditions. The effects of changes in probe temp., ionization potential and instrumental design and geometry were investigated. All of the compds. underwent rearrangement under electron impact, with loss of a neutral mol. of acrylic acid or carboxymethylketene, to form an appropriate secondary amine. The distribution of the total ion current depended on the precise mass spectral condition. Ambiguities in the fragmentation pathways were investigated by high resoln. mass spectrometry.
IT **69241-80-1 69436-77-7 69436-99-3**
RL: PRP (Properties)
(mass spectrum of)
RN 69241-80-1 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



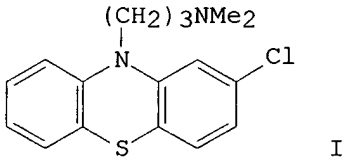
RN 69436-77-7 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



L29 ANSWER 33 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1979:114754 HCAPLUS
DN 90:114754
TI Radioimmunoassay for psychotropic drugs. I. Synthesis and properties of haptens for chlorpromazine
AU Hubbard, J. W.; Midha, K. K.; McGilveray, I. J.; Cooper, J. K.
CS Fac. Pharm., Univ. Manitoba, Winnipeg, Manitoba, Can.
SO J. Pharm. Sci. (1978), 67(11), 1563-71
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal
LA English
GI

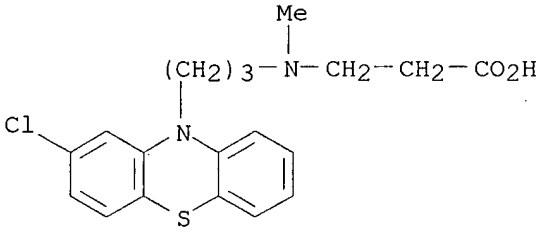


I

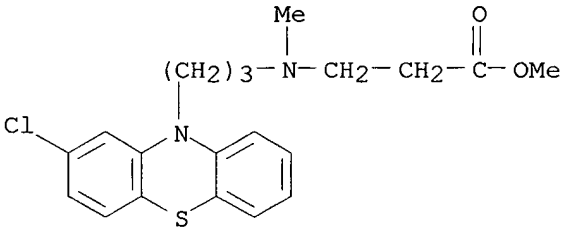
AB For the development of radioimmunoassay procedures for chlorpromazine (I) [50-53-3] and its active metabolites, three I haptens, 7-(3-carboxypropionyl)chlorpromazine [69319-56-8], N-(3-carboxypropionyl)desmethylchlorpromazine [69319-57-9], and N-(2-carboxyethyl)desmethylchlorpromazine [**69436-77-7**], were synthesized and characterized by gas chromatog.-mass spectrometry, proton magnetic resonance spectrometry, and IR spectrophotometry. Each hapten

was coupled to bovine serum albumin, and the no. of hapten residues per mol of bovine serum albumin was calcd. by UV spectrophotometric methods. Antibodies to each hapten-protein conjugate were obtained in rabbits, and titers of the antiserums were checked by evaluating their binding characteristics to 3H-labeled I.

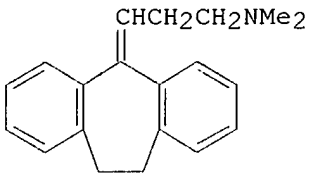
IT **69436-77-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and albumin conjugation of, haptens for radioimmunoassay in relation to)
RN 69436-77-7 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



IT **69319-59-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
RN 69319-59-1 HCAPLUS
CN .beta.-Alanine, N-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



L29 ANSWER 34 OF 34 HCAPLUS COPYRIGHT 2002 ACS
AN 1979:97212 HCAPLUS
DN 90:97212
TI Radioimmunoassay for psychotropic drugs. II. Synthesis and properties of haptens for tricyclic antidepressants
AU Hubbard, J. W.; Midha, K. K.; Cooper, J. K.; Charette, C.
CS Fac. Pharm., Univ. Manitoba, Winnipeg, Manitoba, Can.
SO J. Pharm. Sci. (1978), 67(11), 1571-8
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal
LA English
GI



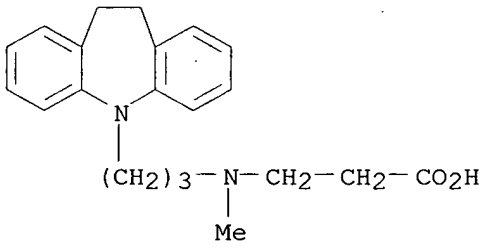
I

AB For the development of radioimmunoassay procedures for tricyclic antidepressants, 2 drug haptens were synthesized for each of a amitriptyline (I) [50-48-6]-nortriptyline [72-69-5] and imipramine [50-49-7]-desipramine [50-47-5] groups. In 1 case, nortriptyline or desipramine was treated with succinic anhydride to yield N-(3-carboxypropionyl) derivs.; in the other case, the haptens were novel N-(2-carboxyethyl) derivs. The hapten and its corresponding ester were characterized by gas-liq. chromatog.-mass spectrometry, proton magnetic resonance spectrometry, and IR spectrophotometry. Each hapten was coupled to bovine serum albumin, and the no. of hapten residues per mol of bovine serum albumin was detd. by UV spectrophotometric methods. Antibodies to each hapten-protein conjugate were developed in rabbits, and titers of the antiserums were checked by evaluating their binding characteristics to tritiated drug.

IT **69241-80-1DP**, serum albumin conjugate **69241-81-2P**
69436-99-3DP, serum albumin conjugate **69437-00-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

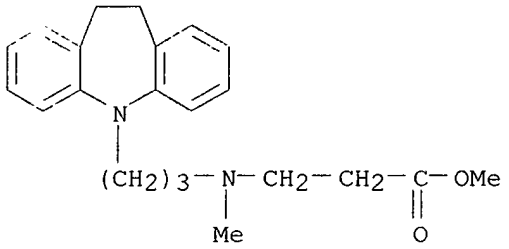
RN 69241-80-1 HCAPLUS

CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)

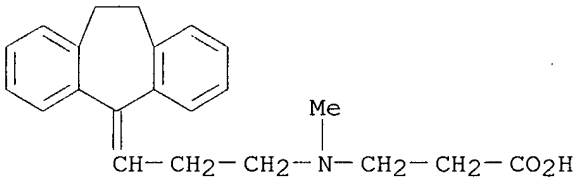


RN 69241-81-2 HCAPLUS

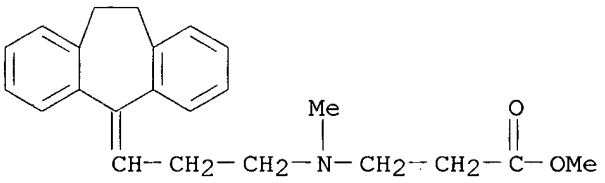
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



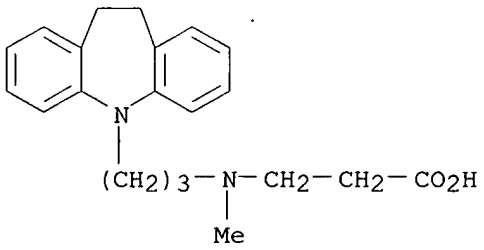
RN 69436-99-3 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 69437-00-9 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



IT **69241-80-1 69436-99-3**
RL: BIOL (Biological study)
(prepn. of an antiserum formation to)
RN 69241-80-1 HCAPLUS
CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenz[b,f]azepin-5-yl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 69436-99-3 HCAPLUS

CN .beta.-Alanine, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)propyl]-N-methyl- (9CI) (CA INDEX NAME)